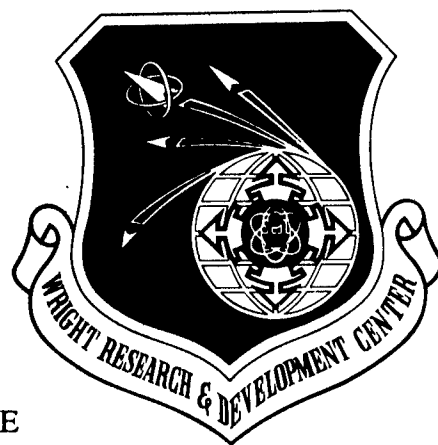


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SINGLE-CRYSTAL DIFFRACTION ANALYSIS OF  
2-(TRIMETHYLSILYLETHYNYL)-4-NITRO-N,N-DIMETHYLANILINE



David A. Grossie  
Department of Chemistry  
Wright State University  
Dayton, Ohio 45435-0001

Albert V. Fratini  
Department of Chemistry  
University of Dayton  
Dayton, Ohio 45469-0001

W. Wade Adams  
Polymer Branch  
Nonmetallic Materials Division

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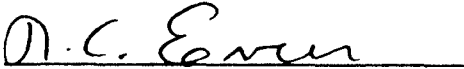
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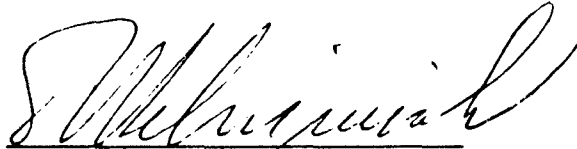
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R. C. EVERS  
Project Scientist  
Nonmetallic Materials Division



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Polymer Branch  
Nonmetallic Materials Division

FOR THE COMMANDER



MERRILL L. MINGES, Director  
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## FOREWORD

This is an interim report on the crystal structure of 2-(Trimethylsilylethynyl)-4-nitro-N,N-dimethylaniline, of interest as an intermediate in the synthesis of materials with potential nonlinear optical properties. The research was conducted between June 1988 and June 1989 by personnel from Wright State University Chemistry Department, from University of Dayton Chemistry Department, and from the Polymer Branch, Materials Laboratory, Wright Research and Development Center. Dr. Grossie's work was sponsored by the WRDC Materials Laboratory through the Summer Faculty Research Program with Universal Energy Systems, Contract F49620-88-C-0053 via a mini-grant with Wright State University. Dr. Fratini's work was sponsored by the WRDC Materials Laboratory through AFOSR Grant 88-0044, with the University of Dayton, Department of Chemistry. The research was performed in the Morphology Laboratory, Polymer Branch, WRDC under the direction of Dr. Wade Adams, Morphology Group Leader, and monitored by Dr. Robert C. Evers, WUD 43 Leader.

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## SECTION I

### INTRODUCTION.

The Polymer Branch of the Materials Laboratory at the Wright Research and Development Center, Wright-Patterson Air Force Base is interested in the synthesis and characterization of polymeric materials. Basic research is also conducted in the structure of polymeric materials and the correlation of the structure and physical properties. The emphasis of this area is to predict the properties of a polymer prior to its synthesis. In this way, the synthesis problem can have greater direction and produce new and better materials with more efficiency. One of the techniques used in determining the structure of polymers is to examine by single-crystal x-ray diffraction methods compounds that may be used to form the backbone, pendants, or cross-links of the polymer. By knowing the structure of a small, repeating portion of the polymer, the polymer itself may be mathematically modeled, yielding the physical properties.

The current study involves the structural analysis of 2-(Trimethylsilylethynyl)-4-nitro-N,N-dimethylaniline by single-crystal x-ray diffraction techniques, with the intent to provide data which may be used to correlate the observed structure and the magnitude of the nonlinear optical response. The primary structural information that is needed by the currently accepted theories is the centricity of the crystal lattice in which the compound of interest crystallizes and the extent of  $\pi$ -orbital conjugation. This compound was selected for study because of its relationship with 2-methyl-4-nitroaniline, a compound with known nonlinear optical properties, and other conjugated systems with separated electron donor and acceptor groups.

## SECTION II

### EXPERIMENTAL METHODS

A yellow rectangular crystal of  $C_{13}H_{18}N_2O_2Si$  was obtained from Bruce Reinhardt of the Polymer Branch, having approximate dimensions of 0.30 x 0.50 x 0.60 mm, was mounted on a glass fiber with its long axis roughly parallel to the  $\phi$  axis of the goniometer. Preliminary examination and data collection were performed with Mo  $K\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ) on an Enraf-Nonius CAD4 computer controlled kappa axis diffractometer equipped with a graphite crystal incident beam monochromator.

Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 23 reflections in the range  $6 < \theta < 12^\circ$ , measured by the computer controlled diagonal slit method of centering. The monoclinic cell parameters and calculated volume are:  $a = 20.258(6)$ ,  $b = 10.444(4)$ ,  $c = 7.129(2) \text{ \AA}$ ,  $\beta = 93.05(2)^\circ$ ,  $V = 1505.9 \text{ \AA}^3$ . For  $Z = 4$  and F.W. = 262.39, the calculated density is  $1.16 \text{ g/cm}^3$ .

The data were collected at a temperature of  $23^\circ$  using the  $\omega/2\theta$  scan technique. The scan rate varied from 0.57 to  $2.79^\circ/\text{min}$  (in omega). The variable scan rate allows rapid data collection for intense reflections where a fast scan rate is used and assures good counting statistics for weak reflections where a slow scan rate is used. Data were collected to a maximum  $2\theta$  of  $64.0^\circ$ . The scan range (in deg.) was determined as a function of  $\theta$  to correct for the separation of the  $K\alpha$  doublet and ranged from 1.21 to 1.41 degrees. Moving-crystal moving-counter background counts were made by scanning an additional 25% above and below this range. Thus the ratio of peak counting time to background counting time was 2:1. The horizontal and vertical counter apertures were set at 2.0 mm and 4.0 mm, respectively. The diameter of the

Table 1. Experimental Details

Formula:	$C_{13}H_{18}N_2O_2Si$
Formula weight:	262.39
F(000):	560
Crystal dim.:	0.30 x 0.50 x 0.60 mm
Radiation:	Mo $K\alpha$
Wavelength:	0.71073 Å
Temperature:	23°
Crystal form:	monoclinic
Space group:	$P2_1/c$
Cell constants:	$a = 20.258(6)$ Å
	$b = 10.444(4)$ Å
	$c = 7.129(2)$ Å
	$\beta = 93.05(2)^\circ$
Volume:	1505.9 Å <sup>3</sup>
Z:	4
Density:	1.16 g/cm <sup>3</sup>
Absorption coeff.:	1.5 cm <sup>-1</sup>
Scan type:	$\omega/2\theta$
Scan rate:	0.57 - 2.79°/min
Scan width:	1.2 + 0.344 tan $\theta$
Maximum 2 $\theta$ :	64.0°
Refl. measured:	5592 total
	5266 unique
Corrections:	Lorentz-polarization
	Reflection averaging (agreement on I = 4.4%)
	Numerical absorption (from 93.29 to 96.06 on I)
	Extinction (coefficient = $1.21 \times 10^{-7}$ )
Observations:	1536 with $F_o^2 > 3\sigma(F_o^2)$
Parameters:	164
R:	0.085
wR:	0.108
Goodness-of-fit:	2.98
Max. shift/error:	0.01
Residual density	
maximum:	0.30(7) e/Å <sup>3</sup>
minimum:	0.27(7) e/Å <sup>3</sup>

incident beam collimator was 0.8 mm and the crystal to detector distance was 21 cm. For intense reflections a Zr metal foil which has an attenuation factor of 12.06 was automatically inserted in front of the detector. The data were examined for systematic absences using the program LOOK (Chapius, 1984), which simulates precession-type photographs. From the observed systematic absences of  $h0l$ ,  $l=2n+1$  and  $0k0$ ,  $k=2n+1$  and from subsequent least-squares refinement, the space group was determined to be  $P2_1/c$  (# 14).

A total of 5592 reflections were collected, of which 5266 were unique and not systematically absent. Lorentz and polarization corrections were applied to the data as well as a numerical absorption correction. The absorption correction used a description of the crystal as being bounded by the  $0,0,1$ ;  $0,0,-1$ ;  $0,-1,1$ ;  $0,1,-1$ ;  $0,1,1$ ;  $0,-1,-1$ ;  $1,0,-1$ ; and  $-1,0,1$  faces with distances from the faces to the centroid of the crystal being 0.02262, 0.00842, 0.02514, 0.02472, 0.02732, 0.02452, 0.03285, and 0.02772 cm, respectively. The linear absorption coefficient is  $1.5 \text{ cm}^{-1}$  for Mo  $K\alpha$  radiation. Relative transmission coefficients ranged from 0.93294 to 0.96061 with an average value of 0.95027. A secondary extinction correction was applied (Zachariasen, 1963). The final coefficient, refined in least-squares, was  $1.21 \times 10^{-7}$  (in absolute units). Intensities of equivalent reflections were averaged, with 24 reflections rejected from the averaging process because their intensities differed significantly from the average. The agreement factors for the averaging of the 44 observed and accepted reflections was 4.4% based on intensity and 4.6% based on  $F_o$ .

The structure was solved by the application of the direct methods program MULTAN (Main, 1982). Using 244 reflections having a minimum normalized structure factor of 2.05, and 1480 triplet relationships, 16 potentially correct phase sets were produced. A total of 18 atoms were

located from an E-map prepared from the phase set with the highest probability of being correct. The remaining non-hydrogen atoms were located in succeeding difference Fourier syntheses using the original 18 to determine the phasing of the observed reflections. Hydrogen atom positions were calculated from geometric considerations and were included in the refinement but restrained to ride on the atom to which each was bonded. The structure was refined by the full-matrix least-squares technique where the function minimized was  $\sum w(|F_o| - |F_c|)^2$  and the weight  $w$  is defined as the reciprocal of the standard deviation on the observed structure factor, squared. Only the 1536 reflections having intensities greater than 3.0 times their standard deviation were used in the refinements. The final cycle of refinement included 164 variable parameters and converged (largest parameter shift was 0.01 times its estimated standard deviation) with unweighted and weighted agreement factors of 0.085 and 0.108, respectively. The standard deviation of an observation of unit weight was 2.98. The highest peak in the final difference Fourier map had a height of  $0.30 \text{ e}/\text{\AA}^3$  and the largest negative peak had a height of  $-0.27 \text{ e}/\text{\AA}^3$ . In each case the height of the peak had an estimated error based on  $\Delta F$  of 0.07 (Cruickshank, 1949). Scattering factors were taken from Cromer and Waber (1974). Anomalous dispersion effects were included in  $F_c$  as described by Ibers and Hamilton (1964); the values for  $\Delta f'$  and  $\Delta f''$  were those of Cromer (1974). All calculations were performed on a VAX computer using SDP/VAX (Frenz, 1978). A summary of experimental details is shown in Table 1. Tables 2 and 3 present the final atomic coordinates and thermal parameters. Derived values in the form of interatomic distances and angles, torsion angles and least-squares planes are tabulated in Tables 4, 5, and 6. Observed and calculated structure factor amplitudes are included as the Appendix.

Table 2. Fractional Coordinates ( $\times 10^4$  for Si, O, N, and C and  $\times 10^3$  for H) and Thermal Parameters for 2-(Trimethylsilylethynyl)-4-nitro-N,N-dimethylaniline.

Atom	x	y	z	B*
Si	0.87838(9)	0.0253(2)	0.3013(3)	6.47(4)
O1	0.6651(2)	0.5391(4)	-0.0576(6)	7.2(1)
O2	0.5645(2)	0.5119(4)	-0.1628(7)	7.6(1)
N1	0.6519(2)	-0.0613(4)	-0.0821(6)	4.9(1)
N4	0.6180(2)	0.4706(4)	-0.1064(6)	5.4(1)
C1	0.6450(2)	0.0688(5)	-0.0848(7)	3.9(1)
C2	0.6973(2)	0.1524(5)	-0.0226(6)	3.6(1)
C3	0.6872(2)	0.2834(5)	-0.0340(6)	3.8(1)
C4	0.6277(2)	0.3328(5)	-0.1008(7)	4.1(1)
C5	0.5755(3)	0.2529(5)	-0.1544(7)	4.6(1)
C6	0.5844(3)	0.1230(5)	-0.1444(7)	4.5(1)
C11	0.5934(3)	-0.1428(6)	-0.1179(9)	6.5(2)
C12	0.7140(3)	-0.1266(6)	-0.105(1)	6.4(2)
C21	0.7575(3)	0.1112(5)	0.0714(7)	4.1(1)
C22	0.8074(3)	0.0842(5)	0.1594(8)	5.1(1)
C23	0.8559(5)	0.009(1)	0.546(1)	13.1(3)
C24	0.9012(5)	-0.1239(9)	0.225(2)	23.5(4)
C25	0.9428(5)	0.139(1)	0.307(2)	18.7(4)
H3	0.724	0.344	0.006	5.0**
H5	0.532	0.290	-0.199	5.0
H6	0.547	0.065	-0.181	5.0
H11a	0.574	-0.128	-0.254	5.0
H11b	0.558	-0.119	-0.023	5.0
H11c	0.606	-0.239	-0.101	5.0
H12a	0.708	-0.194	-0.212	5.0
H12b	0.730	-0.172	0.019	5.0
H12c	0.749	-0.059	-0.140	5.0
H23c	0.817	-0.055	0.554	5.0
H23a	0.896	-0.024	0.630	5.0
H23b	0.842	0.099	0.593	5.0
H24a	0.942	-0.159	0.303	5.0
H24b	0.862	-0.187	0.234	5.0
H24c	0.913	-0.115	0.085	5.0
H25a	0.976	0.119	0.419	5.0
H25b	0.922	0.230	0.326	5.0
H25c	0.967	0.137	0.182	5.0

\*Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:  $(4/3)[a^2B_{11} + b^2B_{22} + c^2B_{33} + ab(\cos\gamma)B_{12} + ac(\cos\beta)B_{13} + bc(\cos\alpha)B_{23}]$

\*\*Thermal parameters on hydrogen atoms were fixed with  $B = 5.0$ .

Table 3. Anisotropic thermal parameters for 2-(Trimethylsilylethynyl)-4-nitro-N,N-dimethylaniline.

Name	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>33</sub>	U <sub>13</sub>	U <sub>23</sub>
Si	0.0575(9)	0.084(1)	0.102(1)	0.0159(9)	-0.0179(9)	0.004(1)
O1	0.101(3)	0.057(2)	0.113(3)	0.005(2)	-0.006(3)	-0.002(2)
O2	0.094(3)	0.076(3)	0.119(3)	0.036(2)	-0.011(3)	0.009(2)
N1	0.065(3)	0.054(3)	0.066(3)	-0.007(2)	0.007(2)	-0.003(2)
N4	0.079(3)	0.064(3)	0.062(3)	0.016(2)	0.004(3)	0.004(2)
C1	0.050(3)	0.057(3)	0.040(3)	-0.003(2)	0.001(2)	0.004(2)
C2	0.043(3)	0.054(3)	0.040(3)	0.001(2)	0.004(2)	0.005(2)
C3	0.053(3)	0.052(3)	0.041(3)	-0.001(2)	0.001(2)	0.002(2)
C4	0.055(3)	0.056(3)	0.043(3)	0.009(3)	0.006(2)	0.004(2)
C5	0.051(3)	0.076(4)	0.048(3)	0.013(3)	-0.005(2)	0.002(3)
C6	0.050(3)	0.069(3)	0.051(3)	-0.004(3)	-0.005(2)	-0.001(3)
C11	0.088(4)	0.062(4)	0.096(5)	-0.024(3)	0.012(4)	-0.011(3)
C12	0.077(4)	0.055(4)	0.111(5)	0.010(3)	0.003(4)	-0.012(3)
C21	0.051(3)	0.050(3)	0.055(3)	-0.002(2)	0.000(2)	-0.002(2)
C22	0.055(3)	0.065(3)	0.071(4)	0.005(3)	-0.005(3)	-0.007(3)
C23	0.161(8)	0.22(1)	0.119(7)	0.064(7)	-0.008(6)	0.045(6)
C24	0.285(8)	0.289(9)	0.30(1)	0.220(6)	-0.182(7)	-0.163(8)
C25	0.136(8)	0.26(1)	0.30(1)	-0.059(8)	-0.111(7)	0.128(9)

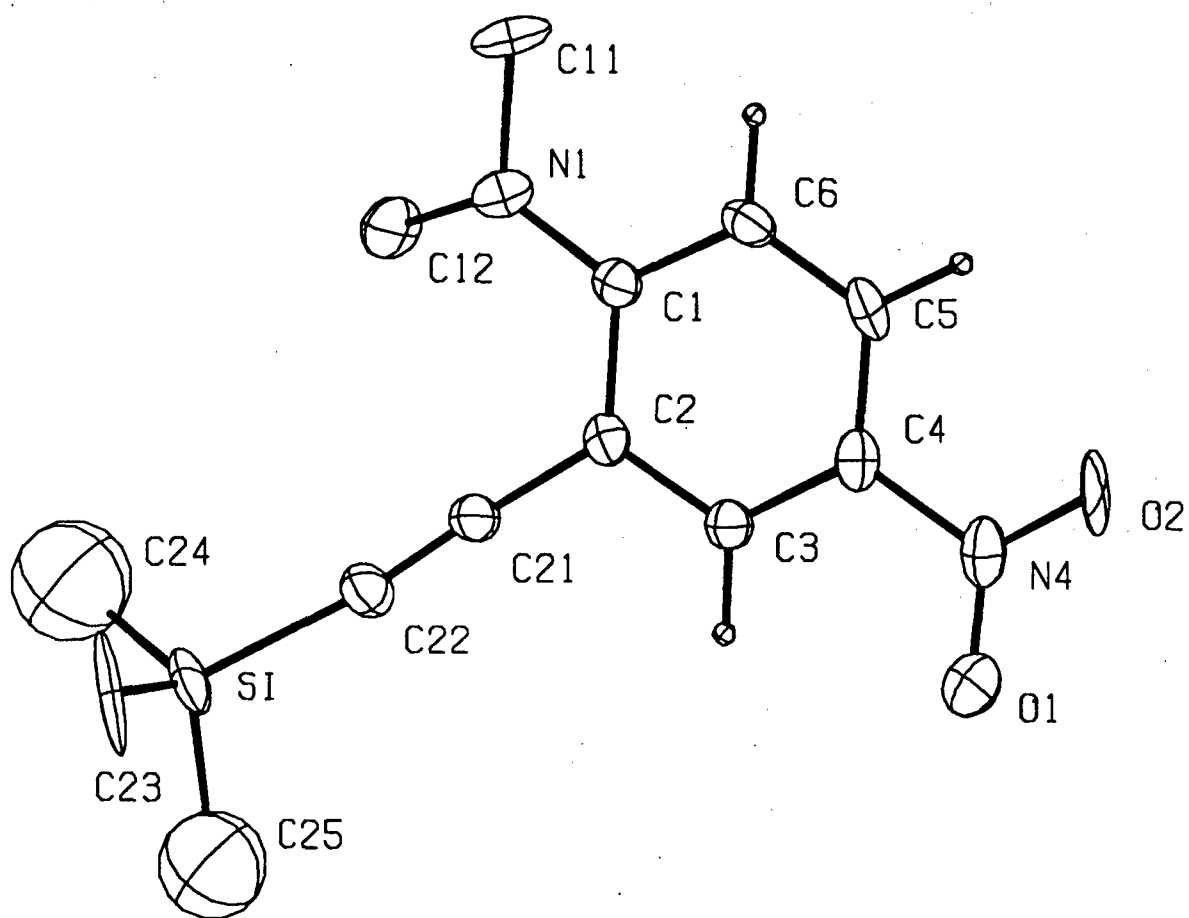
The form of the anisotropic displacement parameter is:

$$\exp[-2\pi^2\{h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2hka^*b^*U_{12} + 2hla^*c^*U_{13} + 2klb^*c^*U_{23}\}]$$

### SECTION III

#### DISCUSSION

Figure 1 shows an ORTEP (Johnson, 1971) drawing of the refined structure of 2-(Trimethylsilylethynyl)-4-nitro-N,N-dimethylaniline. The molecule is essentially planar, with a maximum deviation from planarity of 0.244 Å (see plane 4 in Table 6). The degree of planarity of the central benzene ring, 0.022 Å, is much better (see plane 1 in Table 6). This would indicate that the substituents on the benzene ring do not fit into a common plane as well as the ring itself. The nitro group at the 4-position of the ring is found to be coplanar with the ring, whereas the dimethylamine and trimethylsilylethynyl groups noticeably deviate. The dimethylamine appears to be twisted with respect to the ring, moving C11 and C12, the methyl carbon atoms, 0.138 Å below and 0.655 Å above the plane, respectively. The almost linear trimethylsilylethynyl group is found to extend slightly below the plane of the benzene ring, with deviations of 0.213, 0.446, and 0.892 Å for C21, C22, and Si, respectively. Additionally, this group has distortions in the bond angles at C21 and C22. Normally a carbon-carbon triple bond is linear, with bond angles of 180° at each end, but in the trimethylsilylethynyl group, the bond angles found are 175° and 173°, at C21 and C22, respectively. The bond distances and angles within the benzene ring are reasonable in their regularity, with only one distance, C1-C2, differing greatly from any of the others (1.426 Å vs. 1.371-1.396 Å).



**Figure 1.** ORTEP drawing of 2-(Trimethylsilyl)ethynyl-4-nitro-N,N-Dimethylaniline. Methyl hydrogen atoms have been omitted for clarity.

Table 4. Interatomic Bond Distances (Å) and Angles (°) for 2-(Trimethylsilylethynyl-4-nitro-N,N-dimethylaniline.

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Atom 3	Angle
Si	C22	1.819(6)	C22	Si	C23	109.4(4)
Si	C23	1.832(8)	C22	Si	C24	110.4(4)
Si	C24	1.72(2)	C22	Si	C25	110.1(4)
Si	C25	1.77(1)	C23	Si	C24	107.5(5)
O1	N4	1.227(6)	C23	Si	C25	105.2(5)
O2	N4	1.215(6)	C24	Si	C25	114.1(5)
N1	C1	1.368(7)	C1	N1	C11	119.6(4)
N1	C11	1.471(7)	C1	N1	C12	123.8(4)
N1	C12	1.447(7)	C11	N1	C12	113.8(4)
N4	C4	1.455(7)	O1	N4	O2	123.4(5)
C1	C2	1.426(7)	O1	N4	C4	118.0(4)
C1	C6	1.396(8)	O2	N4	C4	118.6(4)
C2	C3	1.387(7)	N1	C1	C2	122.1(4)
C2	C21	1.425(7)	N1	C1	C6	119.7(5)
C3	C4	1.373(7)	C2	C1	C6	118.1(5)
C4	C5	1.385(7)	C1	C2	C3	118.9(4)
C5	C6	1.371(8)	C1	C2	C21	124.2(4)
C21	C22	1.195(7)	C3	C2	C21	116.5(4)
			C2	C3	C4	121.0(4)
			N4	C4	C3	119.7(4)
			N4	C4	C5	119.4(4)
			C3	C4	C5	120.8(5)
			C4	C5	C6	119.1(5)
			C1	C6	C5	122.0(5)
			C2	C21	C22	175.0(5)
			Si	C22	C21	173.0(6)

Table 5. Torsion Angles (°) for 2-(Trimethylsilylethynyl)-4-nitro-N,N-dimethylaniline.

Atom 1	Atom 2	Atom 3	Atom 4	Angle
C23	Si	C22	C21	-62.02(4.26)
C24	Si	C22	C21	55.97(4.28)
C25	Si	C22	C21	-177.16(4.17)
C11	N1	C1	C2	169.95(0.48)
C11	N1	C1	C6	-8.04(0.71)
C12	N1	C1	C2	-30.38(0.74)
C12	N1	C1	C6	151.64(0.53)
O1	N4	C4	C3	2.91(0.69)
O1	N4	C4	C5	179.81(0.45)
O2	N4	C4	C3	-178.67(0.48)
O2	N4	C4	C5	-1.76(0.71)
N1	C1	C2	C3	178.37(0.44)
N1	C1	C2	C21	-9.20(0.74)
C6	C1	C2	C3	-3.62(0.67)
C6	C1	C2	C21	168.82(0.47)
N1	C1	C6	C5	-178.24(0.47)
C2	C1	C6	C5	3.70(0.74)
C1	C2	C3	C4	1.09(0.69)
C21	C2	C3	C4	-171.93(0.45)
C1	C2	C21	C22	-135.79(6.20)
C3	C2	C21	C22	36.81(6.51)
C2	C3	C4	N4	178.41(0.43)
C2	C3	C4	C5	1.55(0.73)
N4	C4	C5	C6	-178.43(0.45)
C3	C4	C5	C6	-1.55(0.75)
C4	C5	C6	C1	-1.14(0.77)
C2	C21	C22	Si	114.63(6.25)

Table 6. Least-Squares Planes for 2-(Trimethylsilylethynyl)-4-nitro-N,N-dimethylaniline.  
Deviating distances are given in Angstroms.

Orthonormal Equation of Plane 1

$$0.3603 X + 0.0038 Y + -0.9328 Z - 5.2590 = 0$$

$$\text{Chi Squared} = 49.9$$

Defining Atoms

Atom	Distance	Atom	Distance	Atom	Distance	Atom	Distance
C1	0.022(5)	C2	-0.014(5)	C3	-0.004(5)	C4	0.015(5)
C5	-0.006(5)	C6	-0.013(5)				

Orthonormal Equation of Plane 2

$$0.0700 X + -0.8173 Y + -0.5719 Z - -0.2058 = 0$$

$$\text{Chi Squared} = 82.9$$

Defining Atoms

Atom	Distance	Atom	Distance	Atom	Distance	Atom	Distance
C2	-0.016(5)	C21	0.037(5)	C22	-0.022(6)	Si	0.001(2)

Orthonormal Equation of Plane 3

$$-0.0139 X + -0.1165 Y + -0.9931 Z - 0.0000 = 0$$

$$\text{Chi Squared} = 15950.5$$

Defining Atoms

Atom	Distance	Atom	Distance	Atom	Distance	Atom	Distance
C4	0.129(5)	N4	0.004(5)	O1	-0.438(5)	O2	0.367(5)

Table 6 (continued)

Orthonormal Equation of Plane 4

$$0.4673 X + 0.0110 Y + -0.8840 Z - 6.6083 = 0$$

Chi Squared = 21295.1

Defining Atoms

Atom	Distance	Atom	Distance	Atom	Distance	Atom	Distance
C1	0.050(5)	C2	0.153(5)	C3	0.146(5)	C4	0.020(5)
C5	-0.136(5)	C6	-0.131(5)	N1	0.083(4)	N4	-0.019(5)
O1	0.118(5)	O2	-0.156(5)	C21	0.109(5)	C22	0.009(6)
Si	-0.244(2)						

Non-defining atoms

Atom	Distance	Atom	Distance	Atom	Distance	Atom	Distance
C11	-0.248(7)	C12	0.811(7)	C23	-2.039(8)	C24	0.452(12)
C25	0.341(11)						

Dihedral Angles Between Planes:

Plane No.	Plane No.	Dihedral Angle(°)	Plane No.	Plane No.	Dihedral Angle(°)
1	2	56.3(99)	1	3	22.9(1)
1	4	6.8(6)	2	3	48.5(100)
2	4	58.0(96)	3	4	29.5(1)

## SECTION IV

### REFERENCES

Chapius, G., (1984), "LOOK. A FORTRAN Program for Generating Simulated Precession Photographs from Diffractometer Data," University of Lausanne, Switzerland.

Cromer, D. T., (1974), "International Tables for X-Ray Crystallography," Vol. IV, The Kynoch Press, Birmingham, England, Table 2.3.1.

Cromer, D. T. and Waber, J. T., (1974), "International Tables for X-Ray Crystallography," Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2B.

Cruickshank, D. W. J., (1949), Acta Crystallogr., **2**, 154.

Frenz, B.A., (1978), "The Enraf-Nonius CAD-4/SDP--A Real-Time System for Concurrent X-Ray Data Collection and Crystal Structure Determination," Computing in Crystallography, H. Schenk, R. Olthof-Hazelkamp, H. van Konigsveld, and G. C. Bassi, Eds, Delft University Press, Delft, Holland, pp. 64-71.

Ibers, J. A. and Hamilton, W. C., (1964), Acta Crystallogr., **17**, 781.

Johnson, C.K., (1971), ORTEP II. Report ORNL-3794, revised. Oak Ridge National Laboratory, Tennessee.

Main, P., (1982), "MULTAN 11/82. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-Ray Diffraction Data," University of York, England.

Zachariasen, W. H., (1963), Acta Crystallogr., **17**, 781.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
0	0	0	294	246	2	5	0	-10	-7*	0	24	9	0	2	100	113	3
0	0	0	355	349	2	5	0	-8	82	97	4	9	0	4	177	160	3
0	0	0	26*	0	6	5	0	-6	85	90	4	9	0	6	44	39	4
0	0	0	13*	0	16	5	0	-4	699	740	2	9	0	8	47	47	6
0	0	0	-22*	0	17	5	0	-2	436	367	2	10	0	-10	15*	0	22
1	0	-10	22*	0	11	5	0	0	-949*	0	2	10	0	-8	100	111	4
1	0	-8	34*	0	6	5	0	4	140	147	2	10	0	-6	172	183	4
1	0	-6	62	62	3	5	0	4	107	120	3	10	0	-4	144	155	3
1	0	-4	500	451	2	5	0	6	42	58	4	10	0	-2	106	108	3
1	0	-2	556	502	2	5	0	8	-11*	0	20	10	0	0	-244*	0	3
1	0	0	-138*	0	1	5	0	10	-16*	0	19	10	0	2	320	310	2
1	0	0	154	1539	2	5	0	-10	12*	0	14	10	0	4	294	267	3
1	0	4	240	242	3	6	0	-8	93	105	4	10	0	6	29*	0	7
1	0	6	12*	0	16	6	0	-6	178	201	4	10	0	8	13*	0	20
1	0	8	38	24	6	6	0	-4	422	489	3	11	0	-10	-11*	0	25
1	0	10	17*	0	13	6	0	-2	402	440	2	11	0	-8	21*	0	19
2	0	-10	-21*	0	17	6	0	0	644	592	3	11	0	-6	40	31	5
2	0	-8	-35*	0	6	6	0	4	131	128	3	11	0	-4	29*	0	6
2	0	-6	163	164	4	6	0	6	67	68	3	11	0	-2	-38*	0	6
2	0	-4	576	585	6	6	0	8	62	57	4	11	0	0	149	187	4
2	0	-2	2103	2158	3	7	0	-10	-38*	0	13	11	0	2	-66*	0	5
2	0	0	-223*	0	3	7	0	-8	55	59	4	11	0	4	111	115	4
2	0	2	701	670	2	7	0	-6	261	286	3	11	0	6	160	148	4
2	0	4	344	359	6	7	0	-4	324	365	3	12	0	-8	-7*	0	25
2	0	6	31*	0	9	7	0	-2	412	409	4	12	0	-6	54	64	5
2	0	8	-38*	0	12	7	0	0	31	9	3	12	0	-4	13*	0	11
3	0	-10	-8*	0	17	7	0	4	204	207	3	12	0	-2	239	238	3
3	0	-8	16*	0	14	7	0	6	82	84	4	12	0	0	-210*	0	4
3	0	-6	181	207	4	7	0	8	32*	0	18	12	0	2	-102*	0	4
3	0	-4	249	264	3	8	0	-10	42*	0	9	12	0	4	104	100	3
3	0	-2	1847	1908	2	8	0	-8	26*	0	7	12	0	6	46	44	6
3	0	0	-516*	0	3	8	0	-6	197	236	4	13	0	-8	23*	0	18
3	0	2	302	310	2	8	0	-4	217	207	3	13	0	-6	31*	0	6
3	0	4	121	111	3	8	0	-2	32	40	3	13	0	-4	94	86	4
3	0	6	69	73	5	8	0	0	-271*	0	3	13	0	-2	70	65	3
3	0	8	41	37	10	8	0	0	191	191	2	13	0	0	267	302	3
3	0	10	-13*	0	21	8	0	4	123	107	4	13	0	4	440	454	3
4	0	-10	-20*	0	9	8	0	6	94	91	3	13	0	6	23*	0	8
4	0	-8	184	208	3	8	0	8	78	74	4	13	0	8	31*	0	7
4	0	-6	515	551	2	8	0	10	-19*	0	12	13	0	6	-36*	0	12
4	0	-4	204	257	2	9	0	-10	38*	0	8	14	0	-8	-39*	0	11
4	0	-2	20*	0	4	9	0	-8	109	128	4	14	0	-6	17*	0	12
4	0	0	162	158	3	9	0	-6	26*	0	8	14	0	-4	70	94	3
4	0	2	79	81	11	9	0	-4	44	55	4	14	0	-2	-151*	0	4
4	0	4	-13*	0	11	9	0	-2	121	119	3	14	0	0	-198*	0	5
4	0	6	26*	0	10	9	0	0	290	325	2	14	0	2			

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
20	0	-2	155	153	4	27	0	4	-7*	0	23	2	1	-2	472	440	2
20	0	0	9*	0	19	28	0	-4	-27*	0	9	2	1	-1	1066	958	1
20	0	0	-58*	0	0	28	0	-2	-47*	0	10	2	1	0	300	300	1
20	0	4	-37*	0	11	28	0	0	40*	0	7	2	1	1	336	329	1
20	0	6	57*	45	5	28	0	2	-7*	0	26	2	2	1	228	228	2
21	0	-8	-33*	0	18	29	0	-2	-21*	0	19	2	2	1	56	69	2
21	0	-6	22*	0	12	29	0	0	-23*	0	14	2	2	1	77	78	3
21	0	-4	22*	0	9	29	0	2	23*	0	11	3	2	1	41*	0	13
21	0	-2	-78*	0	7	30	0	0	33*	0	8	2	2	1	73	82	3
21	0	0	10*	0	20	0	1	1	11*	0	16	2	2	1	55	41	3
21	0	2	-36*	0	13	0	0	2	209	205	8	2	2	1	37*	0	6
21	0	4	94	77	4	0	0	3	126	129	2	2	2	1	10*	0	4
21	0	6	36*	0	7	0	0	4	61	48	7	2	2	1	19*	0	15
22	0	-6	47*	39	6	0	0	5	135	157	12	3	3	1	-24*	0	16
22	0	-4	0*	0	30	0	0	6	24*	0	6	3	3	1	-17*	0	10
22	0	-2	-9*	0	21	0	0	7	0*	0	21	3	3	1	31*	0	16
22	0	0	39	46	5	0	0	8	23*	0	16	3	3	1	-36*	0	25
22	0	2	-13*	0	21	0	0	9	-20*	0	11	3	3	1	58	76	3
22	0	4	-44*	0	0	0	0	10	21*	0	11	3	3	1	240	275	3
22	0	6	50*	42	6	0	0	11	15*	0	20	3	3	1	123	123	3
23	0	-6	8*	79	25	1	1	-9	11*	0	23	3	3	1	366	340	2
23	0	-4	91	0	15	1	1	-8	-15*	0	11	3	3	1	51	44	3
23	0	-2	-21*	0	0	1	1	-7	13*	0	16	3	3	1	174	172	4
23	0	0	-43*	0	9	1	1	-6	-16*	0	13	3	3	1	62	68	4
23	0	2	-26*	0	17	1	1	-5	18*	0	7	3	3	1	-16*	0	15
23	0	4	-36*	0	11	1	1	-4	-14*	0	11	3	3	1	39	36	7
23	0	6	-24*	0	15	1	1	-3	186	188	2	2	2	1	40*	0	26
24	0	-6	-24*	0	17	1	1	-2	466	385	1	3	3	1	9*	0	13
24	0	-4	8*	0	26	1	1	-1	789	676	1	3	3	1	16*	0	21
24	0	0	-24*	0	13	1	1	0	569	574	1	3	3	1	-9*	0	15
24	0	2	-6*	62	6	1	1	1	314	269	1	3	3	1	-4*	0	4
24	0	4	-13*	0	22	1	1	2	69	80	2	3	3	1	112	128	4
25	0	-6	-10*	0	16	1	1	3	129	134	0	3	3	1	-26*	0	9
25	0	-4	0*	0	32	1	1	4	-23*	0	8	3	3	1	306	305	3
25	0	0	8*	0	22	1	1	5	63	93	4	3	3	1	345	367	2
25	0	2	-51*	0	9	1	1	6	48	50	4	3	3	1	59	51	2
25	0	4	-16*	0	18	1	1	7	37	29	6	3	3	1	42	43	3
25	0	6	46*	36	6	1	1	8	-30*	0	7	3	3	1	131	147	2
26	0	-4	-31*	0	7	1	1	9	-5*	0	18	3	3	1	287	315	2
26	0	-2	16*	0	11	1	1	10	12*	0	14	3	3	1	253	257	3
26	0	0	50	53	6	2	2	-10	-12*	0	21	3	3	1	119	99	3
26	0	2	-58*	0	8	2	2	-8	11*	0	13	3	3	1	-15*	0	11
26	0	4	19*	0	18	2	2	-6	-25*	0	10	3	3	1	-4*	0	14
27	0	-4	-36*	0	11	2	2	-5	34	31	5	3	3	1	-16*	0	14
27	0	-2	8*	0	24	2	2	-3	20*	0	6	3	3	1	44	36	5
27	0	0	-26*	0	15	2	2	-1	94	77	3	3	3	1	25*	0	8
27	0	2	-30*	0	14	2	2	-3	320	366	2	3	3	1	29*	0	9

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
6	1	10	17*	0	20	9	1	5	92	119	4	11	1	3	87	92	4
7	1	9	14*	0	14	9	1	4	-34*	0	7	11	1	4	122	115	4
7	1	8	8*	0	24	9	1	3	160	165	3	11	1	5	32*	0	5
7	1	7	51	55	5	9	1	2	99	76	3	11	1	4	25*	0	7
7	1	6	26*	0	7	9	1	1	165	162	3	11	1	3	60	53	4
7	1	5	25*	0	7	9	1	0	89	88	3	11	1	2	50	45	5
7	1	4	17*	0	14	9	1	1	-16*	0	9	11	1	1	41*	0	7
7	1	3	167	149	3	9	1	2	29	20	3	11	1	0	0	0	25
7	1	2	130	128	3	9	1	1	107	105	3	12	1	1	34*	0	8
7	1	1	-7*	0	12	9	1	4	97	102	4	12	1	0	45	56	5
7	1	0	14*	0	4	9	1	5	162	148	4	12	1	-1	14*	0	11
7	1	-1	136	132	2	9	1	6	103	106	4	12	1	-2	32*	0	12
7	1	-2	316	320	2	9	1	7	-22*	0	13	12	1	-3	-9*	0	16
7	1	-3	-12*	0	9	9	1	8	-24*	0	14	12	1	-4	41	48	3
7	1	-4	170	170	3	9	1	9	29*	0	8	12	1	-5	84	99	4
7	1	-5	55	49	3	10	1	10	32*	0	20	12	1	-6	35	51	4
7	1	-6	133	122	3	10	1	11	4*	0	7	12	1	-7	78	77	3
7	1	-7	75	76	3	10	1	12	33*	0	7	12	1	-8	165	183	3
7	1	-8	66	68	4	10	1	13	-23*	0	8	12	1	-9	311	312	3
7	1	-9	50*	34	6	10	1	14	42	28	4	12	1	0	158	162	4
7	1	-10	-20*	0	16	10	1	15	53	51	3	12	1	1	-25*	0	12
8	1	10	-13*	0	21	10	1	16	52	53	3	12	1	2	26*	28	5
8	1	9	-26*	0	14	10	1	17	-13*	0	6	12	1	3	26*	0	7
8	1	8	54	69	5	10	1	18	169	163	2	12	1	4	29*	0	8
8	1	7	7*	0	23	10	1	19	102	111	3	12	1	5	-25*	0	14
8	1	6	98	109	4	10	1	20	235	256	2	13	1	6	-15*	0	20
8	1	5	73	83	3	10	1	21	35	28	3	13	1	7	10*	0	15
8	1	4	62	71	4	10	1	22	166	155	3	13	1	8	18*	0	10
8	1	3	176	190	3	10	1	23	85	76	4	13	1	9	10*	0	20
8	1	2	35	58	4	10	1	24	110	118	4	13	1	0	44	44	4
8	1	1	21*	31	2	10	1	25	113	109	4	13	1	1	52	52	3
8	1	0	273	268	2	10	1	26	105	102	4	13	1	2	87	84	3
8	1	-1	47	54	2	10	1	27	-27*	0	8	13	1	3	-29*	0	5
8	1	-2	171	166	2	11	1	28	-26*	0	23	13	1	4	-73*	0	7
8	1	-3	26*	84	5	11	1	29	20*	0	17	13	1	5	38	45	4
8	1	-4	86	84	2	11	1	30	42	62	6	13	1	6	182	183	3
8	1	-5	54	47	4	11	1	31	20*	0	18	13	1	7	-39*	0	7
8	1	-6	42	48	6	11	1	32	34*	0	9	13	1	8	70	85	4
8	1	-7	-34*	0	12	11	1	33	53	57	4	13	1	9	83	85	4
8	1	-8	23*	0	11	11	1	34	28*	0	6	13	1	0	232	213	7
8	1	-9	27*	0	10	11	1	35	13*	0	6	13	1	1	33*	0	18
8	1	-10	-49*	0	9	11	1	36	107	86	3	13	1	2	15*	0	19
9	1	10	29*	0	8	11	1	37	111	106	3	13	1	3	-17*	0	15
9	1	9	11*	0	12	11	1	38	12*	0	7	13	1	4	-28*	0	17
9	1	8	100	121	5	11	1	39	273	301	2	14	1	5	-21*	0	8
9	1	7	17*	121	5	11	1	40	59	60	3	14	1	6	31*	0	8

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
16	1	5	11*	0	14	19	1	1	56	107	6	22	1	3	-25*	0	14
16	1	6	17*	0	11	19	1	2	42	48	5	22	1	4	6*	0	17
16	1	7	26*	0	8	19	1	3	-58*	0	7	22	1	5	40*	0	13
16	1	8	-5*	0	17	19	1	4	-9*	0	19	22	1	6	-26*	0	20
17	1	-9	20*	0	12	19	1	5	45	35	5	23	1	-7	15*	0	15
17	1	-8	-17*	0	11	19	1	6	11*	0	20	23	1	-6	-29*	0	24
17	1	-7	13*	0	21	19	1	7	5*	0	19	23	1	-5	8*	0	15
17	1	-6	10*	0	21	20	1	-8	-18*	0	18	23	1	-4	-24*	0	14
17	1	-5	76	67	3	20	1	-7	-23*	0	15	23	1	-3	34*	0	8
17	1	-4	-26*	0	6	20	1	-6	-16*	0	17	23	1	-2	-34*	0	11
17	1	-3	-8*	0	18	20	1	-5	18*	0	14	23	1	-1	51	48	10
17	1	-2	20*	0	17	20	1	-4	-21*	0	14	23	1	0	-35*	0	7
17	1	-1	-122*	0	5	20	1	-3	21*	0	9	23	1	1	47	60	6
17	1	0	169	202	4	20	1	-2	15*	0	24	23	1	2	29*	0	7
17	1	1	213	224	4	20	1	-1	88	132	4	23	1	3	35*	0	7
17	1	2	-61*	62	9	20	1	0	20*	0	5	23	1	4	36*	0	14
17	1	3	91	75	5	20	1	1	35*	0	6	23	1	5	-28*	0	7
17	1	4	148	122	4	20	1	2	122	104	4	24	1	-6	36*	0	8
17	1	5	-22*	0	9	20	1	3	25*	0	8	24	1	-5	22*	0	17
17	1	6	24*	0	9	20	1	4	19*	0	10	24	1	-4	22*	0	11
17	1	7	-7*	0	8	20	1	5	37*	0	7	24	1	-3	-35*	0	21
18	1	-8	-32*	0	12	21	1	-7	24*	0	18	24	1	-2	-6*	0	8
18	1	-7	20*	0	16	21	1	-6	16*	0	19	24	1	-1	-20*	0	15
18	1	-6	17*	0	16	21	1	-5	64	49	4	24	1	0	-17*	0	15
18	1	-5	55	57	4	21	1	-4	49	56	5	24	1	1	43	51	6
18	1	-4	128	137	5	21	1	-3	-35*	0	11	24	1	2	20*	0	16
18	1	-3	-92*	0	6	21	1	-2	-63*	0	11	24	1	3	11*	0	23
18	1	-2	-47*	0	14	21	1	-1	-35*	0	11	24	1	4	8*	0	11
18	1	-1	-130*	0	5	21	1	0	-63*	0	11	24	1	5	19*	0	13
18	1	0	-149*	0	6	21	1	1	10*	0	21	24	1	-6	12*	0	24
18	1	1	14*	0	12	21	1	2	-42*	0	8	25	1	-5	38*	0	8
18	1	2	16*	0	17	21	1	3	30*	0	9	25	1	-4	-35*	0	11
18	1	3	-23*	0	19	21	1	4	-6*	0	22	25	1	-3	-7*	0	23
18	1	4	15*	0	12	21	1	5	22*	0	10	25	1	-2	-33*	0	11
18	1	5	-26*	0	12	21	1	6	30*	0	9	25	1	-1	-21*	0	13
18	1	6	-27*	0	14	21	1	7	-18*	0	8	25	1	0	18*	0	10
18	1	7	36*	0	8	21	1	8	-26*	0	17	25	1	1	-52*	0	9
18	1	8	-33*	0	12	22	1	-6	28*	0	8	25	1	2	31*	0	8
19	1	-7	33*	0	7	22	1	-5	-26*	0	15	25	1	3	30*	0	8
19	1	-6	-24*	0	14	22	1	-4	65	62	4	25	1	4	-44*	0	10
19	1	-5	19*	0	15	22	1	-3	92	95	5	25	1	5	-23*	0	16
19	1	-4	47	50	5	22	1	-2	30*	0	7	26	1	-4	22*	0	24
19	1	-3	52	52	5	22	1	-1	-46*	0	9	26	1	-3	38*	0	16
19	1	-2	140	142	7	22	1	0	-3*	0	17	26	1	-2	21*	0	17
19	1	-1	65	155	7	22	1	1	-62*	0	7	26	1	-1	-38*	0	11
19	1	0	-59*	0	7	22	1	2	0*	0	28	26	1	1	-48*	0	9

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
1	1	1	-17*	0	8	3	3	3	55	50	2	5	2	9	18*	0	19
1	1	2	-2	44	2	3	3	4	70	64	3	5	2	10	12*	0	23
1	1	2	-1	55	2	3	3	5	10*	0	10	6	2	-10	12*	0	24
1	1	2	0	125	2	3	3	6	154	164	4	6	2	-9	-19*	0	17
1	1	2	1	55	2	3	3	7	79	86	4	6	2	-8	-16*	0	10
1	1	2	2	322	2	3	3	8	16*	0	11	6	2	-7	-6*	0	20
1	1	2	3	219	2	3	3	9	23*	0	9	6	2	-6	17*	0	15
1	1	2	4	148	3	3	3	10	-24*	0	15	6	2	-5	43	42	4
1	1	2	5	97	4	3	3	-10	15*	0	14	6	2	-4	182	193	3
1	1	2	6	70	4	3	3	-9	14*	0	13	6	2	-3	225	210	3
1	1	2	7	29*	6	4	4	-8	-12*	0	12	6	2	-2	79	105	3
1	1	2	8	33*	6	4	4	-7	-8*	0	18	6	2	-1	-15*	0	7
1	1	2	9	37*	7	4	4	-6	-27*	0	10	6	2	0	267	247	2
1	1	2	10	-24*	15	4	4	-5	30*	0	5	6	2	1	34	26	2
1	1	2	11	32*	8	4	4	-4	35	38	4	6	2	2	200	225	2
2	2	2	-10	32*	8	4	4	-3	299	273	2	6	2	3	45	21	2
2	2	2	-9	45	5	4	4	-2	102	78	2	6	2	4	360	360	3
2	2	2	-8	7*	20	4	4	-1	83	64	2	6	2	5	133	124	4
2	2	2	-7	88	3	4	4	0	769	796	2	6	2	6	9*	0	18
2	2	2	-6	101	4	4	4	1	255	247	2	6	2	7	31*	0	16
2	2	2	-5	198	3	4	4	2	109	124	2	6	2	8	-17*	0	16
2	2	2	-4	160	3	4	4	3	216	211	2	6	2	9	40*	0	16
2	2	2	-3	328	2	4	4	4	59	78	2	6	2	10	0*	0	32
2	2	2	-2	124	2	4	4	5	36	24	3	6	2	-1	-29*	0	8
2	2	2	-1	63	2	4	4	6	62	59	3	6	2	-2	-23*	0	14
2	2	2	0	277	2	4	4	7	30*	37	5	7	2	-3	17*	0	15
2	2	2	1	260	2	4	4	8	43	0	6	7	2	-4	20*	0	10
2	2	2	2	127	2	4	4	9	-16*	0	19	7	2	-5	29*	0	6
2	2	2	3	341	3	4	4	10	-19*	0	16	7	2	-6	41	44	4
2	2	2	4	168	3	4	4	-10	0*	0	23	7	2	-7	152	151	3
2	2	2	5	47	4	5	5	-9	-7*	0	23	7	2	-8	155	145	3
2	2	2	6	23*	7	5	5	-8	35*	0	6	7	2	-9	378	318	2
2	2	2	7	32*	7	5	5	-7	-39*	0	9	7	2	-10	79	90	2
2	2	2	8	-15*	11	5	5	-6	11*	0	18	7	2	-11	126	117	2
2	2	2	9	-19*	0	5	5	-5	-8*	0	16	7	2	-12	271	248	2
2	2	2	10	-12*	0	5	5	-4	-9*	0	14	7	2	-13	170	162	2
3	3	3	-10	-17*	0	5	5	-3	62	53	3	7	2	-14	14*	0	11
3	3	3	-9	-16*	0	5	5	-2	77	56	3	7	2	-15	56	57	11
3	3	3	-8	-19*	0	5	5	-1	214	205	2	7	2	-16	6*	0	19
3	3	3	-7	31*	13	5	5	0	-23*	0	5	7	2	-17	91	91	4
3	3	3	-6	14*	8	5	5	1	47	45	2	7	2	-18	-22*	0	13
3	3	3	-5	185	3	5	5	2	488	489	2	7	2	-19	-7*	0	15
3	3	3	-4	100	3	5	5	3	146	161	3	7	2	-20	-23*	0	17
3	3	3	-3	459	2	5	5	4	-15*	0	11	7	2	-21	-18*	0	17
3	3	3	-2	276	2	5	5	5	72	77	5	8	2	-22	-28*	0	14
3	3	3	-1	230	2	5	5	6	-25*	0	10	8	2	-23	-9*	0	14
3	3	3	0	433	2	5	5	7	12*	0	18	8	2	-24	-18*	0	10
3	3	3	1	52	54	5	5	8	-29*	0	12	8	2	-25	16*	0	10

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
10	2	2	319	319	3	13	2	-7	28*	0	8	15	2	3	-23*	0	11	18	2	-1	19*	0	18
10	2	3	44	46	3	13	2	-6	26*	0	7	15	2	4	129	111	4	18	2	0	77	89	3
10	2	4	143	133	3	13	2	-5	38	35	5	15	2	5	47	35	5	18	2	1	-20*	0	12
10	2	5	35	24	5	13	2	-4	-24*	0	6	15	2	6	29*	0	8	18	2	2	99	88	3
10	2	6	0*	0	27	13	2	-3	36	29	5	15	2	7	13*	0	13	18	2	3	47	39	4
10	2	7	-6*	0	23	13	2	-2	62	70	3	15	2	8	-25*	0	9	18	2	4	46	46	5
10	2	8	40*	0	6	13	2	-1	41	47	4	16	2	9	36*	0	7	18	2	5	7*	0	23
10	2	9	28*	0	9	13	2	0	275	285	3	16	2	-8	14*	0	21	18	2	6	-17*	0	10
11	2	-9	-17*	0	17	13	2	1	99	115	4	16	2	-7	20*	0	10	18	2	7	-19*	0	16
11	2	-8	-6*	0	23	13	2	2	125	118	3	16	2	8	-17*	0	10	18	2	8	-31*	0	7
11	2	-7	-15*	0	11	13	2	3	115	117	4	16	2	-5	12*	0	18	19	2	-8	19*	0	17
11	2	-6	12*	0	12	13	2	4	122	111	4	16	2	-4	-17*	0	14	19	2	-7	-25*	0	15
11	2	-5	22*	0	8	13	2	5	-15*	0	16	16	2	-3	-18*	0	12	19	2	-6	-20*	0	16
11	2	-4	148	157	4	13	2	6	28*	0	14	16	2	-2	146	138	4	19	2	-5	-19*	0	9
11	2	-3	135	113	3	13	2	7	12*	0	17	16	2	-1	6*	73	3	19	2	-4	14*	0	18
11	2	-2	72	72	2	13	2	8	20*	0	14	16	2	0	68	73	3	19	2	-3	-22*	0	12
11	2	-1	105	86	3	13	2	9	-11*	0	21	16	2	1	140	148	4	19	2	-2	45	38	5
11	2	0	61	71	3	14	2	-9	21*	0	10	16	2	2	169	163	4	19	2	-1	105	118	5
11	2	1	142	139	3	14	2	-8	-18*	0	11	16	2	3	43	43	4	19	2	0	39	125	4
11	2	2	76	77	3	14	2	-7	-25*	0	13	16	2	4	-21*	0	13	19	2	1	60	55	4
11	2	3	8*	0	16	14	2	-6	72	74	4	16	2	5	-9*	0	20	19	2	2	57	54	4
11	2	4	102	100	3	14	2	-5	13*	0	17	16	2	6	41	39	6	19	2	3	68	61	4
11	2	5	100	105	4	14	2	-4	-31*	0	12	16	2	7	-29*	0	12	19	2	4	20*	0	16
11	2	6	-14*	0	15	14	2	-3	-17*	0	17	16	2	8	9*	0	26	19	2	5	58	47	5
11	2	7	35*	0	6	14	2	-2	0*	0	12	17	2	-1	9*	0	16	19	2	6	20*	0	10
11	2	8	14*	0	21	14	2	-1	53	56	8	17	2	-2	22*	0	19	20	2	-7	58*	0	15
11	2	9	-42*	0	12	14	2	0	-31*	0	8	17	2	-3	16*	0	16	20	2	-8	-42*	0	10
12	2	-9	-15*	0	19	14	2	1	74	80	3	17	2	-6	-13*	0	18	20	2	-7	-26*	0	15
12	2	-8	20*	0	10	14	2	2	163	160	3	17	2	-5	-19*	0	13	20	2	-6	22*	0	10
12	2	-7	-10*	0	13	14	2	3	88	90	3	17	2	-4	38	26	5	20	2	-5	12*	0	14
12	2	-6	20*	0	9	14	2	4	5*	0	20	17	2	-3	28*	0	6	20	2	-4	21*	0	9
12	2	-5	51	49	4	14	2	5	54	44	4	17	2	-2	60	76	4	20	2	-3	59	58	4
12	2	-4	104	93	4	14	2	6	52	42	4	17	2	-1	107	98	4	20	2	-2	14*	0	18
12	2	-3	70	78	3	14	2	7	13*	0	13	17	2	0	68	81	3	20	2	-1	-32*	0	6
12	2	-2	327	311	3	14	2	8	20*	0	17	17	2	1	15*	0	16	20	2	0	-48*	0	8
12	2	-1	182	169	3	14	2	9	-22*	0	16	17	2	2	-56*	0	6	20	2	1	-36*	0	9
12	2	0	140	147	3	15	2	-9	-18*	0	18	17	2	3	-19*	0	12	20	2	2	11*	0	12
12	2	1	143	151	3	15	2	-8	-20*	0	10	17	2	4	39	69	3	20	2	3	63	56	4
12	2	2	59	69	3	15	2	-7	25*	0	9	17	2	5	-37*	0	10	20	2	4	-44*	0	9
12	2	3	78	79	3	15	2	-6	39	32	6	17	2	6	31*	0	6	20	2	5	-17*	0	16
12	2	4	44	42	4	15	2	-5	-25*	0	12	17	2	7	-25*	0	14	20	2	6	13*	0	19
12	2	5	93	87	3	15	2	-4	125	122	4	17	2	8	12*	0	22	20	2	7	23*	0	10
12	2	6	107	95	4	15	2	-3	68	47	3	18	2	-8	-11*	0	23	20	2	8	-34*	0	12
12	2	7	-25*	0	13	15	2	-2	13*	0	16	18	2	-7	-12*	0	18	21	2	-7	-41*	0	11
12	2	8	11*	0	22	15	2	-1	31	9	5	18	2	-6	-13*	0	20	21	2	-6	-21*	0	10
12	2	9	-45*	0	10	15	2	0	110	121	4	18	2	-5	-12*	0	17	21	2	-5	-37*	0	10
13	2	-9	-35*	0	7	15	2	1	32*	0	5	18	2	-4	-32*	0	10	21	2	-4	7*	0	16
13	2	-8	19*	0	18	15	2	2	46	56	4	18	2	-3	73	73	3	21	2	-3	68	66	4

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
21	2	-1	43	44	5	24	2	5	-7*	0	22	0	3	3	250	213	36
21	2	0	9*	0	14	25	2	-6	-4*	0	20	0	3	4	162	136	23
21	2	1	-22*	0	12	25	2	-5	-23*	0	15	0	3	5	94	92	7
21	2	2	38*	0	7	25	2	-4	24*	0	9	0	3	6	-11*	0	11
21	2	3	20*	0	9	25	2	-3	22*	0	10	0	3	7	22*	0	11
21	2	4	-39*	0	9	25	2	-2	30*	0	7	0	3	8	21*	0	9
21	2	5	18*	0	10	25	2	-1	15*	0	18	0	3	9	23*	0	25
21	2	6	-38*	0	11	25	2	0	55	48	5	0	3	10	4*	0	20
21	2	7	15*	0	20	25	2	1	41	34	6	0	3	-10	27*	0	9
22	2	-7	18*	0	12	25	2	2	39*	0	7	1	1	3	-37*	0	12
22	2	-6	-43*	0	11	25	2	3	-21*	0	15	1	1	3	29*	0	7
22	2	-5	-16*	0	17	25	2	4	-7*	0	23	1	1	3	30*	0	6
22	2	-4	7*	0	16	25	2	5	-11*	0	14	1	1	3	46	48	4
22	2	-3	-6*	0	24	26	2	-5	-30*	0	14	1	1	3	19*	0	7
22	2	-2	45	56	6	26	2	-4	-27*	0	17	1	1	3	15*	0	6
22	2	-1	0*	0	20	26	2	-3	-18*	0	17	1	1	3	40	33	3
22	2	0	30*	0	7	26	2	-2	8*	0	23	1	1	3	375	316	2
22	2	1	-24*	0	7	26	2	-1	-10*	0	20	1	1	3	67	84	3
22	2	2	30*	0	4	26	2	0	-30*	0	7	1	1	3	19*	0	3
22	2	3	62	51	7	26	2	1	-25*	0	13	1	1	3	470	453	2
22	2	4	-33*	0	11	26	2	2	37*	0	15	1	1	3	37	31	3
22	2	5	9*	0	24	26	2	3	-22*	0	12	1	1	3	127	122	3
22	2	6	-31*	0	14	27	2	4	-33*	0	24	1	1	3	95	87	3
23	2	-7	40*	0	6	27	2	-5	0*	0	12	1	1	3	107	105	4
23	2	-6	-18*	0	17	27	2	-4	-32*	0	12	1	1	3	20*	75	8
23	2	-5	0*	0	30	27	2	-3	-29*	0	13	1	1	3	78	0	3
23	2	-4	46	46	6	27	2	-2	-14*	0	20	1	1	3	-19*	0	16
23	2	-3	-17*	0	17	27	2	-1	-23*	0	9	1	1	3	-37*	0	12
23	2	-2	10*	0	21	27	2	0	-13*	0	18	1	1	3	-19*	0	17
23	2	-1	-11*	0	19	27	2	1	-22*	0	15	2	2	3	-36*	0	6
23	2	0	-21*	0	8	27	2	2	-8*	0	16	2	2	3	-23*	0	14
23	2	1	-38*	0	9	28	2	3	-11*	0	22	2	2	3	-23*	0	8
23	2	2	4*	0	12	28	2	-4	-35*	0	14	2	2	3	23*	0	14
23	2	3	-23*	0	20	28	2	-2	-21*	0	12	2	2	3	29*	0	5
23	2	4	22*	0	15	28	2	-1	-11*	0	16	2	2	3	83	82	4
23	2	5	-26*	0	15	28	2	0	-13*	0	21	2	2	3	405	353	2
24	2	-6	12*	0	24	28	2	1	-11*	0	19	2	2	3	346	302	2
24	2	-5	35*	0	7	28	2	2	-16*	0	20	2	2	3	422	358	2
24	2	-4	-14*	0	19	29	2	3	-12*	0	17	2	2	3	553	532	2
24	2	-3	-31*	0	15	29	2	-2	-16*	0	19	2	2	3	73	80	3
24	2	-2	-17*	0	15	29	2	-1	12*	0	21	2	2	3	237	246	2
24	2	-1	-48*	0	9	29	2	0	7*	0	19	2	2	3	67	69	3
24	2	0	-46*	0	9	29	2	1	-20*	0	17	2	2	3	94	108	4
24	2	1	-10*	0	19	29	2	2	-18*	0	17	2	2	3	29*	0	5
24	2	2	-17*	0	17	29	2	3	692	709	76	2	2	3	73	65	4
24	2	3	-17*	0	17	0	0	3	366	303	56	2	2	3	-8*	0	20
24	2	4				0		2				2	2	3	-11*	0	19

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
5	3	-6	-18*	0	12	7	3	0	284	277	2	9	3	8	16*	0	18
5	3	-5	98	107	4	7	3	1	567	555	2	9	3	9	-20*	0	16
5	3	-4	99	110	4	7	3	2	210	216	2	10	3	-9	14*	0	14
5	3	-3	98	60	3	7	3	3	286	289	3	10	3	-8	-29*	0	12
5	3	-2	279	249	2	7	3	4	49	41	3	10	3	-7	19*	0	16
5	3	-1	41	67	2	7	3	5	18*	0	8	10	3	-6	-16*	0	15
5	3	0	30	44	3	7	3	6	59	64	3	10	3	-5	48*	60	4
5	3	1	47	41	2	7	3	7	12*	0	12	10	3	-4	24*	0	6
5	3	2	145	152	2	7	3	8	8*	0	23	10	3	-3	111	91	4
5	3	3	169	161	3	7	3	9	20*	0	18	10	3	-2	146	138	3
5	3	4	241	263	3	8	3	-10	9*	0	26	10	3	-1	391	361	2
5	3	5	63	59	3	8	3	-9	-33*	0	12	10	3	0	82	59	3
5	3	6	42	42	4	8	3	-8	-26*	0	13	10	3	1	183	186	3
5	3	7	53	51	4	8	3	-7	39	52	6	10	3	2	44	47	3
5	3	8	-14*	0	18	8	3	-6	-8*	0	12	10	3	3	14*	0	12
5	3	9	31*	0	7	8	3	-5	27*	0	6	10	3	4	75	67	3
5	3	10	15*	0	21	8	3	-4	103	101	4	10	3	5	26*	0	6
6	3	-10	12*	0	21	8	3	-3	49	64	3	10	3	6	-10*	0	18
6	3	-9	-21*	0	15	8	3	-2	171	153	3	10	3	7	-21*	0	14
6	3	-8	-24*	0	8	8	3	-1	152	121	2	10	3	8	11*	0	22
6	3	-7	-25*	0	11	8	3	0	20*	0	5	10	3	9	18*	0	12
6	3	-6	-10*	0	17	8	3	1	190	171	3	11	3	-9	-23*	0	17
6	3	-5	51	59	3	8	3	2	278	271	2	11	3	-8	27*	0	8
6	3	-4	76	78	3	8	3	3	186	192	3	11	3	-7	-13*	0	11
6	3	-3	222	188	3	8	3	4	49	53	4	11	3	-6	0*	0	27
6	3	-2	127	127	3	8	3	5	108	108	4	11	3	-5	52	55	4
6	3	-1	544	524	2	8	3	6	0*	0	19	11	3	-4	118	110	4
6	3	0	269	240	2	8	3	7	-25*	0	12	11	3	-3	77	77	4
6	3	1	213	226	2	8	3	8	17*	0	18	11	3	-2	97	95	4
6	3	2	32	29	3	8	3	9	-38*	0	11	11	3	-1	27*	0	5
6	3	3	140	134	3	9	3	-10	14*	0	14	11	3	0	247	251	3
6	3	4	106	94	3	9	3	-9	-17*	0	17	11	3	1	271	262	3
6	3	5	38	40	4	9	3	-8	-34*	0	11	11	3	2	38	53	3
6	3	6	41	34	5	9	3	-7	28*	0	7	11	3	3	56	58	3
6	3	7	-5*	0	15	9	3	-6	38	34	5	11	3	4	65	65	3
6	3	8	8*	0	22	9	3	-5	63	62	3	11	3	5	34	32	5
6	3	9	14*	0	13	9	3	-4	92	93	3	11	3	6	70	71	4
6	3	10	-11*	0	20	9	3	-3	320	294	3	11	3	7	-30*	0	11
7	3	-10	-24*	0	16	9	3	-2	123	114	3	11	3	8	-32*	0	12
7	3	-9	16*	0	18	9	3	-1	53	54	3	11	3	9	15*	0	20
7	3	-8	-22*	0	14	9	3	0	238	272	2	12	3	-9	21*	0	11
7	3	-7	8*	0	15	9	3	1	155	154	3	12	3	-8	11*	0	20
7	3	-6	-26*	0	10	9	3	2	27*	0	4	12	3	-7	-13*	0	18
7	3	-5	49	57	4	9	3	3	47	35	3	12	3	-6	16*	0	10
7	3	-4	-25*	0	10	9	3	4	114	111	4	12	3	-5	71	75	3
7	3	-3	129	123	3	9	3	5	103	94	4	12	3	-4	54	54	3
7	3	-2	119	121	3	9	3	6	11*	0	12	12	3	-3	7*	0	13
7	3	-1	210	193	2	9	3	7	43	40	5	12	3	-2	127	108	3

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
15	3	-9	-21*	0	17	17	3	4	70	52	4	20	3	3	95	85	4	24	3	-4	26*	0	9
15	3	-8	-23*	0	15	17	3	5	60	55	4	20	3	4	25*	0	7	24	3	-3	15*	0	12
15	3	-7	-22*	0	14	17	3	6	-20*	0	9	20	3	5	31*	0	7	24	3	-2	-42*	0	10
15	3	-6	-27*	0	12	17	3	7	18*	0	18	20	3	6	37*	0	6	24	3	-1	15*	0	17
15	3	-5	24*	0	8	17	3	8	-24*	0	9	20	3	7	21*	0	16	24	3	0	44	47	5
15	3	-4	55	57	3	18	3	-8	7*	0	18	21	3	-7	-38*	0	12	24	3	1	48	35	5
15	3	-3	-9*	0	17	18	3	-7	20*	0	14	21	3	-6	-17*	0	11	24	3	2	27*	0	8
15	3	-2	67	60	3	18	3	-6	-23*	0	18	21	3	-5	-17*	0	10	24	3	3	55*	40	5
15	3	-1	53	48	3	18	3	-5	15*	0	11	21	3	-4	7*	0	23	24	3	4	36*	0	6
15	3	0	171	166	3	18	3	-4	-6*	0	21	21	3	-3	39	33	6	24	3	5	-13*	0	18
15	3	1	75	77	3	18	3	-3	22*	0	8	21	3	-2	76	72	4	25	3	-6	-29*	0	14
15	3	2	69	77	3	18	3	-2	50	44	4	21	3	-1	-9*	0	19	25	3	-5	-31*	0	13
15	3	3	79	84	3	18	3	-1	73	77	4	21	3	0	-7*	0	13	25	3	-4	-13*	0	13
15	3	4	-12*	0	16	18	3	0	83	86	3	21	3	1	27*	70	7	25	3	-3	-27*	0	19
15	3	5	-14*	0	15	18	3	1	74	69	3	21	3	2	-37*	0	10	25	3	-2	14*	0	13
15	3	6	-18*	0	9	18	3	2	27*	0	6	21	3	3	-37*	0	7	25	3	-1	26*	0	8
15	3	7	-17*	0	22	18	3	3	-35*	0	9	21	3	4	35*	47	5	25	3	0	-22*	0	15
15	3	8	-25*	0	16	18	3	4	-32*	0	11	21	3	5	12*	0	20	25	3	1	-23*	0	14
16	3	-9	-27*	0	14	18	3	5	37*	0	9	22	3	6	7*	0	18	25	3	2	31*	0	10
16	3	-8	19*	0	11	18	3	6	25*	0	15	22	3	7	14*	0	13	25	3	3	-11*	0	8
16	3	-7	23*	0	8	19	3	-8	-23*	0	9	22	3	-5	34*	0	7	25	3	4	0*	0	31
16	3	-6	50	45	5	19	3	-7	-38*	0	11	22	3	-4	-19*	0	14	26	3	-5	-8*	0	16
16	3	-5	-13*	0	15	19	3	-6	-7*	0	22	22	3	-3	-33*	0	10	26	3	-4	-29*	0	8
16	3	-4	-20*	0	10	19	3	-5	29*	0	7	22	3	-2	18*	0	9	26	3	-3	0*	0	30
16	3	-3	12*	0	16	19	3	-4	-26*	0	26	22	3	-1	75	73	8	26	3	-2	-23*	0	15
16	3	-2	-9*	0	10	19	3	-3	46	48	4	22	3	0	-33*	0	8	26	3	-1	-10*	0	12
16	3	-1	26*	0	7	19	3	-2	-15*	0	15	22	3	1	13*	0	13	26	3	0	0*	0	28
16	3	0	20*	0	8	19	3	-1	30*	0	6	22	3	2	32*	0	11	26	3	1	-7*	0	23
16	3	1	18*	88	4	19	3	0	135	138	4	22	3	3	-38*	0	10	26	3	2	8*	0	24
16	3	2	80	43	5	19	3	1	-21*	0	12	22	3	4	-38*	0	15	26	3	3	15*	0	20
16	3	3	41	48	5	19	3	2	20*	0	10	22	3	5	-38*	0	11	27	3	-4	9*	0	25
16	3	4	51	0	6	19	3	3	-10*	0	21	23	3	-6	13*	0	14	27	3	-3	-32*	0	13
16	3	5	37*	0	9	19	3	4	-20*	0	16	23	3	-5	30*	0	11	27	3	-2	-10*	0	7
16	3	6	24*	0	20	19	3	5	19*	0	18	23	3	-4	8*	0	23	27	3	-1	-27*	0	22
16	3	7	-29*	0	13	19	3	6	-20*	0	21	23	3	-3	21*	0	9	27	3	0	-19*	0	8
16	3	8	17*	0	18	20	3	-7	9*	0	26	23	3	-2	34*	0	7	27	3	1	-17*	0	16
17	3	-8	21*	0	16	20	3	-6	-32*	0	13	23	3	-1	-23*	0	13	27	3	2	-19*	0	23
17	3	-7	41	32	11	20	3	-5	20*	0	10	23	3	0	59	58	4	28	3	-3	-18*	0	18
17	3	-6	-31*	0	7	20	3	-4	18*	0	10	23	3	1	11*	0	20	28	3	-2	-19*	0	11
17	3	-5	-20*	0	4	20	3	-3	-33*	0	8	23	3	2	-40*	0	10	28	3	-1	-38*	0	11
17	3	-4	88	79	20	20	3	-2	27*	0	14	23	3	3	35*	0	6	28	3	0	-5*	0	17
17	3	-3	72	64	3	20	3	-1	-37*	0	9	23	3	4	35*	0	24	28	3	1	25*	0	10
17	3	0	41	51	4	20	3	0	8*	0	14	23	3	5	-39*	0	11	28	3	2	-13*	0	14
17	3	1	12*	0	15	20	3	1	18*	0	15	23	3	6	-39*	0	12	29	3	2	-11*	0	21
17	3	2	48	47	4	20	3	2	-32*	0	10	24	3	-6	-32*	0	25	29	3	3	-29*	0	13
17	3	3	16*	0	15	20	3	3	37*	0	6	24	3	-5	8*	0	8	29	3	3	-29*	0	13

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
29	3	0	12*	0	22	2	4	-2	113	115	3	7	4	-9	-25*	0	8
29	3	1	-33*	0	12	2	4	-1	381	343	2	7	4	-8	-24*	0	13
0	4	0	17*	0	4	2	4	0	260	230	2	7	4	-7	-6*	0	22
0	4	1	100	99	8	2	4	1	91	106	3	7	4	-6	26*	0	7
0	4	2	171	150	19	2	4	2	12*	0	6	7	4	-5	77	84	4
0	4	3	185	167	24	2	4	3	65	90	3	7	4	-4	-20*	0	7
0	4	4	58	68	6	2	4	4	50	45	3	7	4	-3	86	77	4
0	4	5	60	41	3	2	4	5	56	56	3	7	4	-2	214	191	3
0	4	6	16*	0	14	2	4	6	-30*	0	10	7	4	-1	140	146	3
0	4	7	51	49	4	2	4	7	36*	0	6	7	4	0	141	157	3
0	4	8	46	49	4	2	4	8	-12*	0	8	7	4	1	62	67	2
0	4	9	22*	0	8	2	4	9	-29*	0	8	7	4	2	151	161	3
0	4	10	31*	0	6	2	4	10	-7*	0	25	7	4	3	70	67	3
0	4	11	13*	0	12	3	4	-10	-24*	0	15	7	4	4	29*	0	5
0	4	12	-9*	0	13	3	4	-9	12*	0	14	7	4	5	36	43	5
0	4	13	-23*	0	9	3	4	-8	-15*	0	16	7	4	6	67	69	3
0	4	14	-13*	0	20	3	4	-7	-33*	0	10	7	4	7	-13*	0	17
0	4	15	-23*	0	10	3	4	-6	-13*	0	15	7	4	8	49	47	5
0	4	16	0*	0	30	3	4	-5	57	60	3	7	4	9	-51*	0	10
1	4	-10	17*	0	18	3	4	-4	194	161	3	8	4	-10	-38*	0	12
1	4	-9	16*	0	18	3	4	-3	38	18	3	8	4	-9	-24*	0	16
1	4	-8	-24*	0	13	3	4	-2	234	228	2	8	4	-8	26*	0	12
1	4	-7	-17*	0	14	3	4	-1	294	249	2	8	4	-7	22*	0	8
1	4	-6	36	40	5	3	4	0	217	203	2	8	4	-6	30*	0	6
1	4	-5	65	53	3	3	4	1	209	203	2	8	4	-5	-19*	0	12
1	4	-4	47	37	3	3	4	2	37	15	3	8	4	-4	70	83	3
1	4	-3	43	37	3	3	4	3	64	82	3	8	4	-3	337	295	3
1	4	-2	192	190	2	3	4	4	137	140	3	8	4	-2	111	106	3
1	4	-1	540	481	2	3	4	5	35	38	4	8	4	-1	204	210	3
1	4	0	58	73	3	3	4	6	36	42	5	8	4	0	45	43	3
1	4	1	35	40	2	3	4	7	30*	0	6	8	4	1	-20*	0	10
1	4	2	124	139	3	3	4	8	-35*	0	13	8	4	2	-16*	0	13
1	4	3	34	47	3	3	4	9	14*	0	20	8	4	3	33*	0	15
1	4	4	95	98	3	3	4	10	19*	0	18	8	4	4	38*	0	16
1	4	5	48	54	3	3	4	-10	-10*	0	14	8	4	5	-6*	0	17
1	4	6	61	62	3	3	4	-9	-20*	0	16	8	4	6	16*	0	11
1	4	7	-17*	0	15	3	4	-8	35*	0	6	9	4	7	19*	0	9
1	4	8	-24*	0	13	3	4	-7	12*	0	20	9	4	8	44	37	5
1	4	9	-32*	0	12	3	4	-6	-8*	0	18	9	4	9	42	52	5
2	4	-10	33*	0	7	4	4	-5	-6*	0	12	9	4	-10	-21*	0	11
2	4	-9	14*	0	19	4	4	-4	59	47	3	9	4	-9	16*	0	9
2	4	-8	25*	0	8	4	4	-3	333	301	2	9	4	-8	19*	0	5
2	4	-7	23*	0	8	4	4	-2	154	157	2	9	4	-7	44	37	5
2	4	-6	14*	0	15	4	4	-1	68	72	3	9	4	-6	42	52	5
2	4	-5	43	31	4	4	4	0	450	483	2	9	4	-5	-18*	0	11
2	4	-4	186	164	3	4	4	1	78	79	3	9	4	-4	38	40	4
2	4	-3	64	53	2	4	4	2	103	117	3	9	4	-3	-18*	0	11
2	4	-2	64	53	2	4	4	3	57	57	2	9	4	-1	55	45	2

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
9	4	0	338	344	2	12	4	-9	-26*	0	15	14	4	2	-30*	0	9
9	4	1	148	161	3	12	4	-8	18*	0	19	14	4	3	18*	0	8
9	4	2	182	191	3	12	4	-7	18*	0	11	14	4	4	61	60	3
9	4	3	164	168	3	12	4	-6	17*	0	10	14	4	5	17*	0	14
9	4	4	-21*	0	6	12	4	-5	6*	0	21	14	4	6	61	53	4
9	4	5	25*	0	6	12	4	-4	45	57	0	14	4	7	35*	0	7
9	4	6	21*	0	8	12	4	-3	6*	0	20	14	4	8	29*	0	8
9	4	7	-22*	0	13	12	4	-2	164	152	3	15	4	-9	-10*	0	15
9	4	8	-26*	0	13	12	4	-1	98	103	4	15	4	-8	8*	0	25
9	4	9	32*	0	8	12	4	0	111	113	3	15	4	-7	-5*	0	17
10	4	-9	-35*	0	13	12	4	1	126	139	0	15	4	-6	-22*	0	13
10	4	-8	-10*	0	20	12	4	2	12*	0	9	15	4	-5	-18*	0	10
10	4	-7	-27*	0	12	12	4	3	44	61	4	15	4	-4	36	36	5
10	4	-6	-26*	0	11	12	4	4	81	97	3	15	4	-3	39	39	3
10	4	-5	-11*	0	16	12	4	5	51	40	4	15	4	-2	103	96	5
10	4	-4	-17*	0	13	12	4	6	-24*	0	12	15	4	-1	35	40	4
10	4	-3	66	68	3	12	4	7	36*	0	19	15	4	0	53	59	3
10	4	-2	146	135	3	12	4	8	-15*	0	16	15	4	1	31*	0	5
10	4	-1	94	145	3	12	4	9	-24*	0	14	15	4	2	164	165	4
10	4	0	155	177	3	13	4	-9	-22*	0	10	15	4	3	53	55	3
10	4	1	77	75	3	13	4	-8	8*	0	25	15	4	4	40	43	5
10	4	2	159	149	3	13	4	-7	-9*	0	20	15	4	5	56	42	4
10	4	3	87	85	3	13	4	-6	0*	0	6	15	4	6	-8*	0	23
10	4	4	94	100	4	13	4	-5	33*	64	3	15	4	7	-21*	0	15
10	4	5	-22*	101	12	13	4	-4	64	48	3	15	4	8	-44*	0	10
10	4	6	96	101	4	13	4	-3	55	34	3	15	4	9	-15*	0	17
10	4	7	15*	0	11	13	4	-2	34	24	4	16	4	-7	21*	0	10
10	4	8	-7*	0	23	13	4	-1	65	59	2	16	4	-6	-11*	0	18
10	4	9	-13*	0	13	13	4	0	86	83	3	16	4	-5	-17*	0	9
11	4	-9	-16*	0	18	13	4	1	158	161	4	16	4	-4	-33*	0	14
11	4	-8	19*	0	16	13	4	2	85	78	4	16	4	-3	-14*	0	19
11	4	-7	-15*	0	16	13	4	3	139	146	11	16	4	-2	62	48	3
11	4	-6	30*	0	6	13	4	4	9*	0	7	16	4	-1	148	144	4
11	4	-5	100	104	4	13	4	5	23*	0	14	16	4	0	55	62	3
11	4	-4	16*	0	14	13	4	6	-26*	0	13	16	4	1	103	108	4
11	4	-3	22*	0	6	13	4	7	-28*	0	14	16	4	2	9*	0	19
11	4	-2	75	85	3	14	4	8	0*	0	32	16	4	3	-27*	0	12
11	4	-1	76	80	3	14	4	-9	-22*	0	10	16	4	4	61	63	4
11	4	0	72	70	3	14	4	-8	11*	0	22	16	4	5	50	31	5
11	4	1	56	64	3	14	4	-7	-22*	0	14	16	4	6	-20*	0	16
11	4	2	-11*	0	13	14	4	-6	-27*	0	11	16	4	7	29*	0	8
11	4	3	38	43	4	14	4	-5	17*	0	9	17	4	8	12*	0	22
11	4	4	45	32	4	14	4	-4	24*	0	16	17	4	-7	14*	0	20
11	4	5	17*	0	10	14	4	-3	-9*	0	3	17	4	-6	-20*	0	16
11	4	6	36*	0	7	14	4	-2	86	76	13	17	4	-5	-33*	0	10
11	4	7	-13*	0	14	14	4	-1	11*	0	10	17	4	-4	-5*	0	14
11	4	8	17*	0	14	14	4	0	73	88	4	17	4	-3	-16*	0	16
11	4	9	-13*	0	14	14	4	1	0	0	4	17	4	-2	0	0	19

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
20	4	-1	-18*	0	13	23	4	5	-28*	0	13	29	4	0	15*	0	21	2	5	0	316	287	2
20	4	0	-110	105	5	24	4	-6	19*	0	19	0	5	1	689	684	59	2	5	1	46	54	2
20	4	1	-17*	0	14	24	4	-5	-15*	0	19	0	5	2	57	78	5	2	5	2	21*	0	4
20	4	2	92	80	15	24	4	-4	-23*	0	15	0	5	3	247	242	32	2	5	3	195	200	3
20	4	3	19*	0	15	24	4	-3	-33*	0	11	0	5	4	125	112	3	2	5	4	63	54	3
20	4	4	15*	0	19	24	4	-2	-31*	0	11	0	5	4	98	112	4	2	5	4	26*	0	6
20	4	5	-31*	0	12	24	4	-1	-48*	0	9	0	5	5	19*	0	8	2	5	5	-8*	0	18
20	4	6	26*	0	10	24	4	0	40	32	6	0	5	6	7*	0	12	2	5	6	-20*	0	14
20	4	7	12*	0	22	24	4	1	21*	0	16	0	5	7	17*	0	13	2	5	7	-19*	0	15
21	4	-7	-25*	0	15	24	4	2	20*	0	10	0	5	8	-19*	0	13	2	5	8	17*	0	12
21	4	-6	22*	0	10	24	4	3	14*	0	14	0	5	9	-6*	0	14	3	5	9	-30*	0	13
21	4	-5	-10*	0	22	24	4	4	12*	0	14	0	5	10	-33*	0	11	3	5	10	21*	0	16
21	4	-4	-9*	0	20	24	4	5	-16*	0	19	0	5	8	-15*	0	13	3	5	-8	-22*	0	13
21	4	-3	-27*	0	12	25	4	-5	-16*	0	10	0	5	9	-32*	0	18	3	5	-7	-9*	0	20
21	4	-2	38	30	5	25	4	-4	-17*	0	10	0	5	9	-15*	0	13	3	5	-6	51	52	4
21	4	-1	32*	0	6	25	4	-3	-32*	0	10	0	5	10	-16*	0	19	3	5	-5	151	136	4
21	4	0	29*	0	7	25	4	-2	32*	0	8	0	5	10	-32*	0	20	3	5	-4	30*	200	5
21	4	1	19*	0	16	25	4	-1	-9*	0	14	0	5	10	-32*	0	19	3	5	-3	244	44	3
21	4	2	-45*	0	8	25	4	0	-33*	0	12	1	5	-10	-10*	0	8	3	5	-2	47	244	3
21	4	3	52	44	5	25	4	1	26*	0	8	1	5	-9	-12*	0	20	3	5	-1	516	451	2
21	4	4	16*	0	18	25	4	2	-10*	0	21	1	5	-8	0*	0	19	3	5	0	241	235	2
21	4	5	-13*	0	20	25	4	3	39*	0	6	1	5	-7	6*	0	26	3	5	1	154	226	2
21	4	6	40*	0	7	25	4	4	-43*	0	15	1	5	-6	85	90	21	3	5	2	56	68	2
22	4	-7	17*	0	20	26	4	-5	-23*	0	11	1	5	-5	56	25	3	3	5	4	31	12	4
22	4	-6	-29*	0	13	26	4	-4	8*	0	25	1	5	-4	118	99	3	3	5	5	53	51	3
22	4	-5	-16*	0	11	26	4	-3	22*	0	16	1	5	-3	286	265	2	3	5	6	29*	0	6
22	4	-4	45	44	5	26	4	-2	38*	0	7	1	5	-2	59	33	2	3	5	7	18*	0	12
22	4	-3	47	38	5	26	4	-1	32*	0	9	1	5	-1	423	416	2	3	5	8	-19*	0	10
22	4	-2	-21*	0	9	26	4	0	22*	0	7	1	5	0	49	53	2	3	5	9	18*	0	18
22	4	-1	16*	0	17	26	4	1	42*	0	21	1	5	1	220	205	2	4	5	-10	15*	0	20
22	4	0	21*	0	10	26	4	2	-23*	0	14	1	5	2	68	73	3	4	5	-9	19*	0	17
22	4	1	66	49	4	26	4	3	15*	0	20	1	5	3	38	74	3	4	5	-8	36	23	5
22	4	2	11*	0	20	27	4	4	-25*	0	19	1	5	4	-26*	50	5	4	5	-6	-21*	0	12
22	4	3	50*	0	17	27	4	-3	-13*	0	8	1	5	5	18*	0	10	4	5	-5	76	61	3
22	4	4	0*	0	31	27	4	-2	-17*	0	17	1	5	6	-35*	0	17	4	5	-4	121	111	4
22	4	5	-52*	0	15	27	4	-1	-25*	0	30	1	5	7	-38*	0	11	4	5	-3	257	220	3
23	4	-6	-25*	0	19	27	4	0	17*	0	18	2	5	8	-28*	0	16	4	5	-2	86	58	3
23	4	-5	-14*	0	19	27	4	1	-20*	0	17	2	5	-10	41	39	18	4	5	-1	261	230	2
23	4	-4	19*	0	16	27	4	2	-41*	0	11	2	5	-8	17*	0	19	4	5	0	114	116	3
23	4	-3	42	38	6	28	4	-3	-44*	0	9	2	5	-6	-5*	0	19	4	5	1	123	133	3
23	4	-2	13*	0	20	28	4	-2	13*	0	13	2	5	-5	42	42	4	4	5	2	-18*	0	10
23	4	-1	71	60	4	28	4	-1	-44*	0	9	2	5	-4	438	375	3	4	5	3	80	89	3
23	4	0	32*	0	7	28	4	0	16*	0	12	2	5	-3	21*	0	16	4	5	4	37	38	5
23	4	1	-6*	0	22	28	4	1	-37*	0	12	2	5	-2	407	351	2	4	5	5	-30*	0	10
23	4	2	-21*	0	16	28	4	2	-37*	0	12	2	5	-1									
23	4	3	60*	50	5	29	4	-1			12	2	5										

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
4	5	8	17*	0	11	7	5	-1	110	103	3	12	5	0	53	49	3
4	5	9	-10*	0	21	7	5	0	288	287	2	12	5	1	31	30	5
5	5	-9	25*	0	9	10	5	-8	122	127	3	12	5	2	138	127	4
5	5	-8	14*	0	12	10	5	-7	172	160	3	12	5	3	27*	0	6
5	5	-7	41	38	5	10	5	-6	167	174	3	12	5	4	75	71	3
5	5	-6	-7*	0	13	10	5	-5	62	54	3	12	5	5	48	45	4
5	5	-5	168	149	4	10	5	-4	0	0	24	12	5	6	13*	0	18
5	5	-4	118	122	4	10	5	-3	-32*	0	10	12	5	7	31*	0	7
5	5	-3	184	167	3	10	5	-2	-28*	0	12	12	5	8	10*	0	21
5	5	-2	150	156	3	10	5	-1	-28*	0	14	10	5	-9	21*	0	18
5	5	-1	62	95	2	9	10	0	-22*	0	15	10	5	-8	-38*	0	11
5	5	0	20*	0	5	10	5	1	-25*	0	15	10	5	-7	-31*	0	12
5	5	1	100	108	3	10	5	2	11*	0	21	10	5	-6	7*	0	23
5	5	2	103	108	3	10	5	3	38*	0	6	10	5	-5	20*	0	8
5	5	3	16*	99	12	10	5	4	54	67	4	10	5	-4	27*	0	6
5	5	4	90	99	14	10	5	5	92	89	4	10	5	-3	69	64	3
5	5	5	15*	0	14	10	5	6	43	36	4	10	5	-2	136	132	4
5	5	6	26*	0	12	10	5	7	11*	0	10	10	5	-1	27*	0	6
5	5	7	-11*	0	13	10	5	8	63	73	5	10	5	0	94	95	4
5	5	8	-14*	0	15	10	5	9	111	104	3	11	5	1	-27*	0	9
5	5	9	-24*	0	13	10	5	-1	25*	0	4	11	5	2	120	125	4
6	6	-9	-10*	0	22	11	5	-8	223	209	3	11	5	-7	62	64	3
6	6	-8	66	55	4	11	5	-6	135	123	4	11	5	-5	-29*	0	12
6	6	-7	22*	0	7	11	5	-5	-13*	0	16	11	5	-4	-24*	0	13
6	6	-6	36	29	5	11	5	-4	24*	0	8	11	5	-3	-21*	0	17
6	6	-5	74	59	3	11	5	-3	45	50	5	11	5	-2	-16*	0	12
6	6	-4	234	209	3	11	5	-2	-14*	0	12	11	5	-1	-12*	0	13
6	6	-3	320	293	3	11	5	-1	23*	0	10	11	5	0	-25*	0	13
6	6	-2	220	237	2	11	5	0	36*	0	7	11	5	1	-33*	0	12
6	6	-1	213	212	2	11	5	1	-30*	0	12	11	5	2	-45*	0	8
6	6	0	193	200	3	11	5	2	24*	0	9	11	5	3	30*	0	16
6	6	1	14*	0	11	11	5	-7	-6*	0	21	11	5	-6	3*	0	12
6	6	2	14*	0	7	11	5	-6	-6*	0	5	11	5	-5	-8*	0	16
6	6	3	14*	46	3	11	5	-5	34	31	5	11	5	-4	52	66	3
6	6	4	-20*	0	11	11	5	-4	155	158	4	11	5	-3	63	54	3
6	6	5	-16*	0	14	11	5	-3	89	74	3	11	5	-2	87	89	3
6	6	6	30*	0	7	11	5	-2	21*	0	6	11	5	-1	75	80	3
6	6	7	19*	0	11	11	5	-1	152	154	3	11	5	0	-20*	0	12
6	6	8	-19*	0	17	12	5	0	-6*	0	16	12	5	1	55	65	4
6	6	9	18*	0	19	12	5	1	56	56	5	12	5	2	-13*	0	9
7	7	-9	-26*	0	13	12	5	-8	-10*	0	13	12	5	-7	-20*	0	17
7	7	-8	12*	0	15	12	5	-6	29*	0	5	12	5	-6	8*	0	24
7	7	-7	149	149	11	12	5	-5	46	51	4	12	5	-4	-20*	0	16
7	7	-6	-22*	0	11	12	5	-4	68	79	4	12	5	-3	9*	0	23
7	7	-5	-22*	0	11	12	5	-3	60	50	4	12	5	-2	-41*	0	11
7	7	-4	9*	0	16	12	5	-2	-8*	0	14	12	5	-1	-12*	0	18
7	7	-3	129	138	3	12	5	-1	-17*	0	10	12	5	0	23*	0	8

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
15	5	-5	-23*	0	13	18	5	-6	17*	0	11	21	5	-2	-27*	0	12
15	5	-4	-8*	0	18	18	5	-5	-9*	0	13	21	5	-1	27*	0	7
15	5	-3	-14*	0	14	18	5	-4	14*	0	16	21	5	0	8*	0	14
15	5	-2	46	48	4	18	5	-3	27*	0	7	21	5	1	53	45	4
15	5	-1	28*	0	6	18	5	-2	56	63	4	21	5	2	58	45	4
15	5	0	75	80	4	18	5	-1	-8*	0	19	21	5	3	-10*	0	18
15	5	1	-16*	0	12	18	5	0	37	34	5	21	5	4	-37*	0	10
15	5	2	60	56	3	18	5	1	85	79	4	21	5	5	21*	0	11
15	5	3	79	86	4	18	5	2	-31*	0	10	21	5	6	31*	0	8
15	5	4	-17*	0	14	18	5	3	57	58	4	22	5	-6	0*	0	31
15	5	5	61	58	4	18	5	4	27*	0	7	22	5	-5	20*	0	17
15	5	6	-21*	0	15	18	5	5	-35*	0	10	22	5	-4	11*	0	22
15	5	7	-15*	0	11	18	5	6	-30*	0	12	22	5	-3	-10*	0	20
15	5	8	-21*	0	16	18	5	7	-35*	0	12	22	5	-2	29*	0	7
16	5	-7	-24*	0	15	19	5	-6	-50*	0	10	22	5	-1	26*	0	8
16	5	-6	-15*	0	11	19	5	-5	-23*	0	15	22	5	0	37*	0	6
16	5	-5	32*	0	7	19	5	-4	14*	0	19	22	5	1	-12*	0	11
16	5	-4	26*	0	13	19	5	-3	44	54	5	22	5	2	43*	0	18
16	5	-3	39	34	5	19	5	-2	-28*	0	11	22	5	3	-31*	0	25
16	5	-2	-8*	0	18	19	5	-1	53	46	4	22	5	4	-8*	0	18
16	5	-1	29*	0	16	19	5	0	44	54	5	23	5	-5	-48*	0	9
16	5	0	-18*	0	13	19	5	1	80	71	5	23	5	-6	9*	0	17
16	5	1	87	94	4	19	5	2	42	38	6	23	5	-4	18*	0	18
16	5	2	34*	0	6	19	5	3	37*	0	19	23	5	-3	30*	0	13
16	5	3	38	28	5	19	5	4	-14*	0	19	23	5	-2	-26*	0	11
16	5	4	-30*	0	12	19	5	5	-37*	0	12	23	5	-1	41	40	6
16	5	5	26*	0	8	19	5	6	-11*	0	21	23	5	0	-29*	0	14
16	5	6	12*	0	14	20	5	-7	-31*	0	13	23	5	1	58	47	5
17	5	-7	15*	0	13	20	5	-6	0*	0	30	23	5	2	-17*	0	20
17	5	-6	20*	0	17	20	5	-5	-36*	0	16	23	5	3	14*	0	19
17	5	-5	-32*	0	10	20	5	-4	-5*	0	10	23	5	4	-23*	0	15
17	5	-4	-11*	0	12	20	5	-3	48	43	5	24	5	-5	9*	0	25
17	5	-3	44	43	5	20	5	-2	20*	0	8	24	5	-4	-32*	0	11
17	5	-2	59	54	4	20	5	-1	16*	0	16	24	5	-3	-29*	0	13
17	5	-1	48	55	4	20	5	0	12*	0	17	24	5	-2	19*	0	10
17	5	0	-28*	0	10	20	5	1	17*	0	11	24	5	-1	8*	0	23
17	5	1	18*	0	14	20	5	2	22*	0	9	24	5	0	35*	0	19
17	5	2	7*	0	21	20	5	3	-6*	0	15	24	5	1	-12*	0	9
17	5	3	-21*	0	13	20	5	4	55	51	5	24	5	2	50*	0	38
17	5	4	38	28	5	20	5	5	11*	0	22	24	5	3	50*	0	6
17	5	5	-26*	0	12	21	5	-7	-11*	0	10	25	5	-4	-18*	0	17
17	5	6	21*	0	10	21	5	-6	24*	0	21	25	5	-5	-19*	0	17
17	5	7	-15*	0	20	21	5	-5	-10*	0	21	25	5	-4	14*	0	21
18	5	-8	-29*	0	8	21	5	-4	-27*	0	13	25	5	-3	31*	0	8
18	5	-7	-9*	0	15	21	5	-3	-23*	0	13	25	5	-2	31*	0	20

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
1	1	6	-1	7*	10	3	6	9	22*	0	11	6	6	0	73	66	3
1	1	6	0	25*	4	4	6	-9	-11*	0	14	6	6	1	33	35	4
1	1	6	1	184	3	4	6	-8	-22*	0	9	9	6	-7	45	39	5
1	1	6	2	147	3	4	6	-7	29*	0	7	9	6	-6	25*	0	8
1	1	6	3	80	3	4	6	-6	-24*	0	13	9	6	-5	0*	0	20
1	1	6	4	76	3	4	6	-5	-24*	0	12	9	6	-4	-17*	0	7
1	1	6	5	47	3	4	6	-4	28*	0	6	9	6	-3	-16*	0	8
1	1	6	6	15*	4	4	6	-3	84	82	4	9	6	-2	123	117	4
1	1	6	7	-30*	15	4	6	-2	21*	0	5	9	6	-1	42	49	4
1	1	6	8	7*	12	4	6	-1	221	218	3	9	6	0	40	33	4
1	1	6	9	13*	17	4	6	0	182	174	3	9	6	1	114	113	4
2	2	6	-9	-10*	14	4	6	1	223	224	3	9	6	2	109	113	4
2	2	6	-8	-32*	22	4	6	2	165	169	3	9	6	3	158	164	4
2	2	6	-7	-35*	12	4	6	3	47	31	3	9	6	4	86	82	3
2	2	6	-6	-19*	9	4	6	4	-17*	0	12	9	6	5	21*	0	8
2	2	6	-5	41	14	4	6	5	60	69	0	9	6	6	41	38	6
2	2	6	-4	138	4	4	6	6	15*	0	16	9	6	7	-10*	0	13
2	2	6	-3	136	3	4	6	7	-13*	0	17	9	6	8	-17*	0	18
2	2	6	-2	8*	10	4	6	8	11*	0	22	9	6	9	25*	0	9
2	2	6	-1	38	3	4	6	9	-21*	0	16	10	6	-9	-27*	0	16
2	2	6	0	95	3	5	6	-9	32*	0	7	10	6	-8	-27*	0	14
2	2	6	1	82	3	5	6	-8	36	35	5	10	6	-7	-11*	0	19
2	2	6	2	91	3	5	6	-7	19*	0	15	10	6	-6	-31*	0	9
2	2	6	3	12*	13	5	6	-6	28*	0	6	10	6	-5	36	25	4
2	2	6	4	24*	6	5	6	-5	22*	0	6	10	6	-4	62	61	3
2	2	6	5	-9*	17	5	6	-4	19*	0	6	10	6	-3	45	49	4
2	2	6	6	50	4	5	6	-3	22*	0	3	10	6	-2	54	53	3
2	2	6	7	20*	5	5	6	-2	71	63	2	10	6	-1	52	46	3
2	2	6	8	20*	10	5	6	-1	69	81	3	10	6	0	136	146	4
2	2	6	9	22*	17	5	6	0	134	124	3	10	6	1	114	118	4
3	3	6	-9	-26*	15	5	6	1	104	98	3	10	6	2	-12*	0	15
3	3	6	-8	-48*	11	5	6	2	162	164	5	10	6	3	59	50	4
3	3	6	-7	-12*	14	5	6	3	122	129	4	10	6	4	81	83	3
3	3	6	-6	19*	14	5	6	4	73	79	3	10	6	5	78	80	4
3	3	6	-5	34	15	5	6	5	54	46	4	10	6	6	16*	0	11
3	3	6	-4	193	3	5	6	6	26*	0	4	10	6	7	-39*	0	11
3	3	6	-3	116	3	5	6	7	15*	0	20	11	6	8	34*	0	17
3	3	6	-2	108	3	5	6	8	24*	0	10	11	6	-9	-21*	0	17
3	3	6	-1	38	3	6	6	-9	23*	0	9	11	6	-7	20*	0	17
3	3	6	0	89	3	6	6	-8	-16*	0	11	11	6	-6	-9*	0	20
3	3	6	1	23*	5	6	6	-7	18*	0	16	11	6	-5	34*	0	6
3	3	6	2	69	3	6	6	-6	143	138	4	11	6	-4	-27*	0	10
3	3	6	3	-5*	19	6	6	-5	52	54	3	11	6	-3	-17*	0	13
3	3	6	4	0*	26	6	6	-4	47	51	4	11	6	-2	134	137	4
3	3	6	5	32*	6	6	6	-3	37	20	15	11	6	-1	90	87	4
3	3	6	6	19*	16	6	6	-2	24*	0	22	11	6	0	76	73	3
3	3	6	7	31*	8	6	6	-1	24*	0	5	11	6	1	53	55	3

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
11	6	2	66	72	3	14	6	-2	42	38	4	17	6	-3	54	60	4
11	6	3	37	34	5	14	6	-1	111	105	4	17	6	-2	7*	0	14
11	6	4	7*	0	21	14	6	0	11*	0	10	17	6	-1	40	32	5
11	6	5	68	65	4	14	6	1	11*	0	10	17	6	0	-22*	0	13
11	6	6	-17*	0	16	14	6	2	-20*	95	13	17	6	1	104	107	4
11	6	7	-23*	0	14	14	6	3	96	46	4	17	6	2	83	80	4
11	6	8	-25*	0	15	14	6	4	50	46	5	17	6	3	38	32	6
12	6	-9	22*	0	11	14	6	5	22*	0	9	17	6	4	15*	48	5
12	6	-7	-21*	0	10	14	6	6	-10*	0	20	17	6	5	15*	0	12
12	6	-6	-11*	0	13	14	6	7	8*	0	23	17	6	6	21*	0	10
12	6	-5	-19*	0	15	14	6	8	-7*	0	24	17	6	7	16*	0	19
12	6	-4	-18*	0	15	15	6	-8	15*	0	22	18	6	-7	-16*	0	13
12	6	-3	-10*	0	17	15	6	-7	19*	0	11	18	6	-6	17*	0	18
12	6	-2	-14*	0	15	15	6	-6	13*	0	20	18	6	-5	21*	0	22
12	6	-1	28*	0	16	15	6	-5	14*	0	18	18	6	-4	-10*	0	4
12	6	0	-16*	0	13	15	6	-4	19*	0	16	18	6	-3	60	57	4
12	6	1	196	202	3	15	6	-3	11*	0	20	18	6	-2	23*	0	9
12	6	2	188	178	3	15	6	-2	142	136	4	18	6	-1	7*	0	21
12	6	3	35	48	5	15	6	-1	118	113	4	18	6	0	60	47	3
12	6	4	55	60	4	15	6	0	14*	0	15	18	6	1	20*	0	9
12	6	5	-8*	0	4	15	6	1	71	76	3	18	6	2	46	35	5
12	6	6	11*	0	13	15	6	2	66	76	3	18	6	3	59	54	4
12	6	7	-28*	0	12	15	6	3	-39*	0	9	18	6	4	-3*	0	17
12	6	8	-41*	0	10	15	6	4	-37*	0	9	18	6	5	43	27	5
13	6	-7	-34*	0	12	15	6	5	42	33	5	18	6	6	15*	0	13
13	6	-6	0*	0	22	15	6	6	0*	0	29	18	6	7	29*	0	8
13	6	-5	45	41	5	15	6	7	19*	0	11	19	6	8	12*	0	15
13	6	-4	13*	0	11	15	6	-8	-24*	0	16	19	6	-6	30*	0	19
13	6	-3	57	63	3	16	6	-5	21*	0	10	19	6	-4	22*	0	9
13	6	-2	57	55	3	16	6	-4	41	33	5	19	6	-3	53	58	5
13	6	-1	88	84	4	16	6	-3	23*	0	8	19	6	-2	26*	0	7
13	6	0	112	113	4	16	6	-2	19*	0	15	19	6	-1	0*	0	26
13	6	1	66	67	4	16	6	-1	63	71	3	19	6	0	7*	0	22
13	6	2	102	98	4	16	6	0	15*	0	17	19	6	1	-6*	0	22
13	6	3	-13*	0	17	16	6	1	67	65	3	19	6	2	-14*	0	14
13	6	4	-19*	0	15	16	6	2	18*	0	14	19	6	3	18*	0	18
13	6	5	-26*	0	12	16	6	3	-20*	0	9	19	6	4	-17*	0	12
13	6	6	-27*	0	15	16	6	4	-16*	0	14	20	6	5	0*	0	32
13	6	7	-33*	0	13	16	6	5	21*	0	10	20	6	6	10*	0	16
13	6	8	-40*	0	9	16	6	6	-38*	0	8	20	6	-7	-23*	0	7
14	6	-7	23*	0	10	17	6	-8	30*	0	12	20	6	-6	-27*	0	8
14	6	-6	16*	0	17	17	6	-7	-38*	0	7	20	6	-5	59	48	4
14	6	-5	85	87	3	17	6	-6	32*	0	5	20	6	-4	39	43	6
14	6	-4	77	71	3	17	6	-5	48	44	5	20	6	-3	0	0	0
14	6	-3	0	0	3	17	6	-4	0	0	7	20	6	-2	0	0	0
14	6	-2	0	0	3	17	6	-3	0	0	8	20	6	-1	0	0	0
14	6	-1	0	0	3	17	6	-2	0	0	8	20	6	0	0	0	0
14	6	0	0	0	3	17	6	-1	0	0	7	20	6	1	0	0	0
14	6	1	0	0	3	17	6	0	0	0	5	20	6	2	0	0	0
14	6	2	0	0	3	17	6	1	0	0	5	20	6	3	0	0	0
14	6	3	0	0	3	17	6	2	0	0	5	20	6	4	0	0	0
14	6	4	0	0	3	17	6	3	0	0	5	20	6	5	0	0	0
14	6	5	0	0	3	17	6	4	0	0	5	20	6	6	0	0	0
14	6	6	0	0	3	17	6	5	0	0	5	20	6	7	0	0	0
14	6	7	0	0	3	17	6	6	0	0	5	20	6	8	0	0	0
14	6	8	0	0	3	17	6	7	0	0	5	20	6	9	0	0	0
14	6	9	0	0	3	17	6	8	0	0	5	20	6	10	0	0	0
14	6	10	0	0	3	17	6	9	0	0	5	20	6	11	0	0	0
14	6	11	0	0	3	17	6	10	0	0	5	20	6	12	0	0	0
14	6	12	0	0	3	17	6	11	0	0	5	20	6	13	0	0	0
14	6	13	0	0	3	17	6	12	0	0	5	20	6	14	0	0	0
14	6	14	0	0	3	17	6	13	0	0	5	20	6	15	0	0	0
14	6	15	0	0	3	17	6	14	0	0	5	20	6	16	0	0	0
14	6	16	0	0	3	17	6	15	0	0	5	20	6	17	0	0	0
14	6	17	0	0	3	17	6	16	0	0	5	20	6	18	0	0	0
14	6	18	0	0	3	17	6	17	0	0	5	20	6	19	0	0	0
14	6	19	0	0	3	17	6	18	0	0	5	20	6	20	0	0	0
14	6	20	0	0	3	17	6	19	0	0	5	20	6	21	0	0	0
14	6	21	0	0	3	17	6	20	0	0	5	20	6	22	0	0	0
14	6	22	0	0	3	17	6	21	0	0	5	20	6	23	0	0	0
14	6	23	0	0	3	17	6	22	0	0	5	20	6	24	0	0	0
14	6	24	0	0	3	17	6	23	0	0	5	20	6	25	0	0	0
14	6	25	0	0	3	17	6	24	0	0	5	20	6	26	0	0	0
14	6	26	0	0	3	17	6	25	0	0	5	20	6	27	0	0	0
14	6	27	0	0	3	17	6	26	0	0	5	20	6	28	0	0	0
14	6	28	0	0	3	17	6	27	0	0	5	20	6	29	0	0	0
14	6	29	0	0	3	17	6	28	0	0	5	20	6	30	0	0	0
14	6	30	0	0	3	17	6	29	0	0	5	20	6	31	0	0	0
14	6	31	0	0	3	17	6	30	0	0	5	20	6	32	0	0	0
14	6	32	0	0	3	17	6	31	0	0	5	20	6	33	0	0	0
14	6	33	0	0	3	17	6	32	0	0	5	20	6	34	0	0	0
14	6	34	0	0	3	17	6	33	0	0	5	20	6	35	0	0	0
14	6	35	0	0	3	17	6	34	0	0	5	20	6	36	0	0	0
14	6	36	0	0	3	17	6	35	0	0	5	20	6	37	0	0	0
14	6	37	0	0	3	17	6	36	0	0	5	20	6	38	0	0	0
14	6	38	0	0	3	17	6	37	0	0	5	20	6	39	0	0	0
14	6	39	0	0	3	17	6	38	0	0	5	20	6	40	0	0	0
14	6	40	0	0	3	17	6	39	0	0	5	20	6	41	0	0	0
14	6	41	0	0	3	17	6	40	0	0	5	20	6	42	0	0	0
14	6	42	0	0	3	17	6	41	0	0	5	20	6	43	0	0	0
14	6	43	0	0	3	17	6	42	0	0	5	20	6	44	0	0	0
14	6	44	0	0	3	17	6	43	0	0	5	20	6	45	0	0	0
14	6	45	0	0	3	17	6	44	0	0	5	20	6	46	0	0	0
14	6	46	0	0	3	17	6	45	0	0	5	20	6	47	0	0	0
14	6	47	0	0	3	17	6	46	0	0	5	20	6	48	0	0	0
14	6	48	0	0	3	17	6	47	0	0	5	20	6	49	0	0	0
14	6	49	0	0	3	17	6	48	0	0	5	20	6	50	0	0	0
14	6	50	0	0	3	17	6	49	0	0	5	20	6	51	0	0	0
14	6	51	0	0	3	17	6	50	0	0	5	20	6	52	0	0	0
14	6	52	0	0	3	17	6	51	0	0	5	20	6	53	0	0	0
14	6	53	0	0	3	17	6	52	0	0	5	20	6	54	0	0	0
14	6	54	0	0	3	17	6	53	0	0							

H	K	L	H	K	L	H	K	L	H	K	L	H	K	L	H	K	L	H	K	L	Fobs	Fcalc	SigF	SigF	Fobs	Fcalc	SigF
24	6	2	1	7	2	1	7	2	1	7	2	1	7	2	1	7	2	1	7	2	26*	0	5	14	-25*	0	0
24	6	3	1	7	3	1	7	3	1	7	3	1	7	3	1	7	3	1	7	3	23*	0	6	18	38	30	202
24	6	4	1	7	4	1	7	4	1	7	4	1	7	4	1	7	4	1	7	4	78	68	3	0	9*	0	147
25	6	-4	1	7	5	1	7	5	1	7	5	1	7	5	1	7	5	1	7	5	33*	0	6	115	11	57	132
25	6	-3	1	7	6	1	7	6	1	7	6	1	7	6	1	7	6	1	7	6	18*	0	10	0	-28*	0	0
25	6	-2	1	7	7	1	7	7	1	7	7	1	7	7	1	7	7	1	7	7	66	72	4	44	42	0	0
25	6	-1	1	7	8	1	7	8	1	7	8	1	7	8	1	7	8	1	7	8	23*	0	10	89	-7*	0	0
25	6	0	1	7	9	1	7	9	1	7	9	1	7	9	1	7	9	1	7	9	19*	0	18	98	-37*	0	0
25	6	1	2	7	-9	2	7	-9	2	7	-9	2	7	-9	2	7	-9	2	7	-9	-38*	0	13	152	37*	0	0
25	6	2	2	7	-8	2	7	-8	2	7	-8	2	7	-8	2	7	-8	2	7	-8	-23*	0	6	81	24*	0	0
25	6	3	2	7	-7	2	7	-7	2	7	-7	2	7	-7	2	7	-7	2	7	-7	37*	0	6	30*	18*	0	0
26	6	-3	2	7	-6	2	7	-6	2	7	-6	2	7	-6	2	7	-6	2	7	-6	44	27	5	36	68	0	0
26	6	-2	2	7	-5	2	7	-5	2	7	-5	2	7	-5	2	7	-5	2	7	-5	35	34	5	29	72	0	0
26	6	-1	2	7	-4	2	7	-4	2	7	-4	2	7	-4	2	7	-4	2	7	-4	27*	0	6	46	32*	0	0
26	6	0	2	7	-3	2	7	-3	2	7	-3	2	7	-3	2	7	-3	2	7	-3	9*	0	12	74	203	88	0
26	6	1	2	7	-2	2	7	-2	2	7	-2	2	7	-2	2	7	-2	2	7	-2	21*	0	6	70	158	193	0
26	6	2	2	7	-1	2	7	-1	2	7	-1	2	7	-1	2	7	-1	2	7	-1	87	83	3	0	121	170	0
26	6	3	2	7	0	2	7	0	2	7	0	2	7	0	2	7	0	2	7	0	165	162	3	0	135	170	0
27	6	-1	2	7	1	2	7	1	2	7	1	2	7	1	2	7	1	2	7	1	24*	0	5	-39*	30*	0	0
27	6	0	2	7	2	2	7	2	2	7	2	2	7	2	2	7	2	2	7	2	165	182	3	0	42	20	0
27	6	1	2	7	3	2	7	3	2	7	3	2	7	3	2	7	3	2	7	3	128	133	4	0	98	112	0
27	6	2	2	7	4	2	7	4	2	7	4	2	7	4	2	7	4	2	7	4	34	31	5	0	40	47	0
27	6	3	2	7	5	2	7	5	2	7	5	2	7	5	2	7	5	2	7	5	34*	0	5	42	112	0	0
0	7	1	2	7	6	2	7	6	2	7	6	2	7	6	2	7	6	2	7	6	47	48	5	0	11	112	0
0	7	2	2	7	7	2	7	7	2	7	7	2	7	7	2	7	7	2	7	7	17*	0	5	91	18*	0	0
0	7	3	2	7	8	2	7	8	2	7	8	2	7	8	2	7	8	2	7	8	47	0	6	22*	18*	0	0
0	7	4	2	7	9	2	7	9	2	7	9	2	7	9	2	7	9	2	7	9	17*	0	11	91	19*	0	0
0	7	5	2	7	-9	2	7	-9	2	7	-9	2	7	-9	2	7	-9	2	7	-9	-24*	0	25	125	29*	0	0
0	7	6	2	7	-8	2	7	-8	2	7	-8	2	7	-8	2	7	-8	2	7	-8	-25*	0	10	128	8*	0	0
0	7	7	2	7	-7	2	7	-7	2	7	-7	2	7	-7	2	7	-7	2	7	-7	-46*	0	10	161	-15*	0	0
0	7	8	2	7	-6	2	7	-6	2	7	-6	2	7	-6	2	7	-6	2	7	-6	17*	0	18	132	6*	0	0
0	7	9	2	7	-5	2	7	-5	2	7	-5	2	7	-5	2	7	-5	2	7	-5	0*	0	21	144	11*	0	0
0	7	0	3	7	-4	3	7	-4	3	7	-4	3	7	-4	3	7	-4	3	7	-4	61	61	3	0	55	53	0
0	7	1	3	7	-3	3	7	-3	3	7	-3	3	7	-3	3	7	-3	3	7	-3	-19*	0	13	27*	73	71	0
0	7	2	3	7	-2	3	7	-2	3	7	-2	3	7	-2	3	7	-2	3	7	-2	10*	0	11	0	32*	0	0
0	7	3	3	7	-1	3	7	-1	3	7	-1	3	7	-1	3	7	-1	3	7	-1	25*	0	5	0	41	17	0
0	7	4	3	7	0	3	7	0	3	7	0	3	7	0	3	7	0	3	7	0	64	47	3	0	200	211	0
0	7	5	3	7	1	3	7	1	3	7	1	3	7	1	3	7	1	3	7	1	100	102	4	0	262	273	0
0	7	6	3	7	2	3	7	2	3	7	2	3	7	2	3	7	2	3	7	2	153	156	3	0	164	173	0
0	7	7	3	7	3	3	7	3	3	7	3	3	7	3	3	7	3	3	7	3	49	54	3	0	37	22	0
0	7	8	3	7	4	3	7	4	3	7	4	3	7	4	3	7	4	3	7	4	27*	0	5	0	17*	0	0
0	7	9	3	7	5	3	7	5	3	7	5	3	7	5	3	7	5	3	7	5	38	39	5	0	16*	0	0
0	7	0	3	7	6	3	7	6	3	7	6	3	7	6	3	7	6	3	7	6	120	130	4	0	28*	0	0
0	7	1	3	7	7	3	7	7	3	7	7	3	7	7	3	7	7	3	7	7	87	90	3	0	27*	0	0
0	7	2	3	7	8	3	7	8	3	7	8	3	7	8	3	7	8	3	7	8	-12*	0	21	42	15*	0	0
0	7	3	3	7	9	3	7	9	3	7	9	3	7	9	3	7	9	3	7	9	35	40	5	0	28*	0	0
0	7	4	3	7	-9	3	7	-9	3	7	-9	3	7	-9	3	7	-9	3	7	-9	120	130	4	0	27*	0	0
0	7	5	3	7	-8	3	7	-8	3	7	-8	3	7	-8	3	7	-8	3	7	-8	87	90	3	0	28*	0	0
0	7	6	3	7	-7	3	7	-7	3	7	-7	3	7	-7	3	7	-7	3	7	-7	-12*	0	21	42	15*	0	0
0	7	7	3	7	-6	3	7	-6	3	7	-6	3	7	-6	3	7	-6	3	7	-6	35	40	5	0	27*	0	0
0	7	8	3	7	-5	3	7	-5	3	7	-5	3	7	-5	3	7	-5	3	7	-5	120	130	4	0	28*	0	0
0	7	9	3	7	-4	3	7	-4	3	7	-4	3	7	-4	3	7	-4	3	7	-4	87	90	3	0	28*	0	0
0	7	0	3	7	-3	3	7	-3	3	7	-3	3	7	-3	3	7	-3	3	7	-3	-12*	0	21	42	15*	0	0
0	7	1	3	7	-2	3	7	-2	3	7	-2	3	7	-2	3	7	-2	3	7	-2	35	40	5	0	27*	0	0
0	7	2	3	7	-1	3	7	-1	3	7	-1	3	7	-1	3	7	-1	3	7	-1	120	130	4	0	28*	0	0
0	7	3	3	7	0	3	7	0	3	7	0	3	7	0	3	7	0	3	7	0	87	90	3	0	28*	0	0
0	7	4	3	7	1	3	7	1	3	7	1	3	7	1	3	7	1	3	7	1	-12*	0	21	42	15*	0	0
0	7	5	3	7	2	3	7	2	3	7	2	3	7	2	3	7	2	3	7	2	35	40	5	0	27*	0	0
0	7	6	3	7	3	3	7	3	3	7	3	3	7	3	3	7	3	3	7	3	120	130	4	0	28*	0	0
0	7	7	3	7	4	3	7	4	3	7	4	3	7	4	3	7	4	3	7	4	87	90	3	0	28*	0	0
0	7	8	3	7	5	3	7	5	3	7	5	3	7	5	3	7	5	3	7	5	-12*	0	21	42	15*	0	0
0	7	9	3	7	-9	3	7	-9	3	7	-9	3	7	-9	3	7	-9	3	7	-9	35	40	5	0	27*	0	0
0	7	0	3	7	-8	3	7	-8	3	7	-8	3	7	-8	3	7	-8	3	7	-8	120	130	4	0	28*	0	0
0	7	1	3	7	-7	3	7	-7	3	7	-7	3	7	-7	3	7	-7	3	7	-7	87	90	3	0	28*	0	0
0	7	2	3	7	-6	3	7	-6	3	7	-6	3	7	-6	3	7	-6	3	7	-6	-12*	0	21	42	15*	0	0
0	7	3	3	7	-5	3	7	-5	3	7	-5	3	7	-5	3	7	-5	3	7	-5	35	40	5	0	27*	0	0
0	7	4	3	7	-4	3	7	-4	3	7	-4	3	7	-4	3	7	-4	3	7	-4	120	130	4	0	28*	0	0
0	7	5	3	7	-3	3	7	-3	3	7	-3	3	7	-3	3	7	-3	3	7	-3	87	90	3	0	28*	0	0
0	7	6	3	7	-2	3	7																				

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
9	7	-4	17*	0	14	12	7	-7	19*	0	16	14	7	7	-17*	0	11	18	7	-5	32*	0	8
9	7	-3	81	79	4	12	7	-6	-9*	0	20	15	7	-8	-7*	0	25	18	7	-4	47	37	5
9	7	-2	-16*	0	13	12	7	-5	42	50	6	15	7	-7	-7*	0	26	18	7	-3	15*	0	18
9	7	-1	217	223	3	12	7	-4	-16*	0	10	15	7	-6	-6*	0	17	18	7	-2	58	57	4
9	7	0	103	89	4	12	7	-3	150	149	4	15	7	-5	77	72	4	18	7	-1	-27*	0	11
9	7	1	119	114	4	12	7	-2	132	120	4	15	7	-4	75	63	4	18	7	0	-10*	0	12
9	7	2	139	145	4	12	7	-1	44	32	5	15	7	-3	58	50	4	18	7	1	-21*	0	8
9	7	3	155	171	4	12	7	0	42	10	4	15	7	-2	49	44	4	18	7	2	37	17	6
9	7	4	135	128	4	12	7	1	85	89	3	15	7	-1	-18*	0	13	18	7	3	8*	0	23
9	7	5	12*	0	18	12	7	2	161	164	4	15	7	0	90	87	3	18	7	4	17*	0	16
9	7	6	62	65	4	12	7	3	17*	0	8	15	7	1	54	52	4	18	7	5	20*	0	16
9	7	7	-33*	0	12	12	7	4	72	76	4	15	7	2	53	46	4	18	7	6	19*	0	11
9	7	8	-27*	0	14	12	7	5	56	41	4	15	7	3	28*	0	4	19	7	7	23*	0	13
10	7	-8	22*	0	17	12	7	6	-17*	0	15	15	7	4	55	41	4	19	7	-6	15*	0	10
10	7	-7	13*	0	19	12	7	7	-18*	0	11	15	7	5	20*	0	15	19	7	-5	22*	0	20
10	7	-6	-21*	0	11	12	7	8	-23*	0	22	15	7	6	6*	0	17	19	7	-4	37*	0	14
10	7	-5	-13*	0	9	12	7	-7	15*	0	11	15	7	7	12*	0	22	19	7	-3	-9*	0	20
10	7	-4	84	87	3	13	7	-6	-19*	0	11	16	7	-7	-12*	0	20	19	7	-2	-22*	0	13
10	7	-3	73	74	3	13	7	-5	0*	0	30	16	7	-6	-28*	0	14	19	7	-1	-21*	0	4
10	7	-2	98	101	4	13	7	-4	23*	0	9	16	7	-5	13*	0	20	19	7	0	62	57	4
10	7	-1	140	139	4	13	7	-3	-8*	0	21	16	7	-4	-24*	0	13	19	7	1	59	58	4
10	7	0	103	105	4	13	7	-2	53	54	4	16	7	-3	91	96	3	19	7	2	72	52	4
10	7	1	210	211	4	13	7	-1	82	87	3	16	7	-2	76	65	3	19	7	3	-12*	0	18
10	7	2	56	66	4	13	7	0	174	170	4	16	7	-1	27*	0	6	19	7	4	18*	0	10
10	7	3	69	69	3	13	7	1	122	112	4	16	7	0	-16*	0	14	19	7	5	23*	0	10
10	7	4	37	31	5	13	7	2	20*	0	10	16	7	1	12*	0	18	19	7	6	25*	0	9
10	7	5	-28*	0	13	13	7	3	-18*	0	13	16	7	2	80	77	3	20	7	-6	-23*	0	17
10	7	6	14*	0	19	13	7	4	73	76	4	16	7	3	41	41	6	20	7	-5	-7*	0	23
10	7	7	21*	0	17	13	7	5	-6*	0	9	16	7	4	-24*	0	13	20	7	-4	17*	0	15
10	7	8	-19*	0	12	13	7	6	-26*	0	14	16	7	5	10*	0	15	20	7	-3	20*	0	22
11	7	-7	-30*	0	17	13	7	7	-18*	0	17	16	7	6	18*	0	12	20	7	-2	7*	0	15
11	7	-6	21*	0	17	13	7	8	-20*	0	11	16	7	-7	43*	0	7	20	7	-1	31*	0	7
11	7	-5	59	52	4	14	7	-8	42*	0	11	17	7	-6	43*	0	6	20	7	0	13*	0	12
11	7	-4	54	39	4	14	7	-7	23*	0	12	17	7	-5	-10*	0	22	20	7	1	29*	0	12
11	7	-3	73	76	3	14	7	-6	-33*	0	12	17	7	-4	31*	0	7	20	7	2	-21*	0	9
11	7	-2	54	48	4	14	7	-5	58	65	5	17	7	-3	-27*	0	13	20	7	3	21*	0	16
11	7	-1	100	97	4	14	7	-4	-13*	0	19	17	7	-2	-13*	0	16	20	7	4	24*	0	9
11	7	0	259	261	4	14	7	-3	-15*	0	17	17	7	-1	-14*	0	15	21	7	5	-10*	0	15
11	7	1	162	162	4	14	7	-2	107	102	4	17	7	0	-19*	0	17	21	7	-6	20*	0	18
11	7	2	49	45	4	14	7	-1	78	78	3	17	7	1	-16*	0	16	21	7	-5	20*	0	16
11	7	3	79	69	3	14	7	0	34	37	5	17	7	2	19*	0	15	21	7	-4	30*	0	7
11	7	4	17*	0	15	14	7	1	61	53	3	17	7	3	30*	0	15	21	7	-3	-20*	0	14
11	7	5	32*	0	6	14	7	2	-17*	0	14	17	7	4	-22*	0	13	21	7	-2	-26*	0	13
11	7	6	37*	0	16	14	7	3	-22*	0	8	17	7	5	-42*	0	9	21	7	-1	-17*	0	15
11	7	7	21*	0	11	14	7	4	30*	0	6	17	7	6	-30*	0	13	21	7	0	19*	0	18
11	7	8	18*	0	11	14	7	5	38*	0	6	18	7	7	21*	0	11	21	7	1	24*	0	15
12	7	-8	22*	0	18	14	7	6	-19*	0	14	18	7	-6	48*	31	5	21	7	2	-20*	0	15

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
21	7	4	44*	38	6	0	8	4	38	20	5	2	8	9	15*	0	21
21	7	5	-15*	0	12	0	8	5	53	46	4	3	8	-9	-20*	0	19
21	7	-5	18*	0	17	0	8	5	56	46	4	3	8	-8	17*	0	13
22	7	-4	-26*	0	15	0	8	6	48	43	5	3	8	-7	56	44	5
22	7	-3	27*	0	8	0	8	6	20*	0	17	3	8	-6	45	29	5
22	7	-2	19*	0	10	0	8	7	54	55	5	3	8	-5	61	53	4
22	7	-1	34*	0	7	0	8	7	57	55	5	3	8	-4	24*	0	7
22	7	0	42	35	6	0	8	8	-7*	0	26	3	8	-3	51	42	4
22	7	1	33*	0	6	0	8	8	9*	0	19	3	8	-2	37	29	4
22	7	2	-18*	0	17	0	8	9	7*	0	19	3	8	-1	99	92	4
22	7	3	-26*	0	14	0	8	9	-18*	0	22	3	8	0	122	127	4
22	7	4	-34*	0	13	1	8	-9	-14*	0	22	3	8	1	67	54	3
22	7	5	-14*	0	20	1	8	-8	-40*	0	11	3	8	2	85	99	4
23	7	-5	20*	0	11	1	8	-7	66	59	5	3	8	3	-30*	0	10
23	7	-4	-19*	0	18	1	8	-6	69	61	4	3	8	4	61	65	4
23	7	-3	-7*	0	25	1	8	-5	63	66	4	3	8	5	52	45	4
23	7	-2	11*	0	21	1	8	-4	78	71	4	3	8	6	44	47	6
23	7	-1	25*	0	29	1	8	-3	29*	0	5	3	8	7	22*	0	17
23	7	0	-12*	0	13	1	8	-2	39	39	4	4	8	-9	-15*	0	32
23	7	1	43*	31	6	1	8	1	45	50	17	4	8	-8	-40*	0	11
23	7	2	-21*	0	10	1	8	2	171	193	4	4	8	-6	27*	0	7
24	7	-4	-20*	0	10	1	8	3	120	132	4	4	8	-5	-38*	0	8
24	7	-3	26*	0	9	1	8	4	40	34	5	4	8	-4	23*	0	6
24	7	-2	19*	0	16	1	8	5	42	36	5	4	8	-3	29*	0	5
24	7	-1	-20*	0	11	1	8	6	-17*	0	18	4	8	-2	27*	0	5
24	7	0	-34*	0	12	1	8	7	-26*	0	15	4	8	-1	69	71	3
24	7	1	55*	33	5	1	8	8	17*	0	20	4	8	0	250	279	3
24	7	2	-13*	0	21	1	8	9	42*	0	20	4	8	1	204	215	3
25	7	-3	-25*	0	15	2	8	-8	20*	0	11	4	8	2	97	98	3
25	7	-2	21*	0	11	2	8	-6	49	42	5	4	8	3	57	61	4
25	7	-1	-27*	0	14	2	8	-5	79	72	3	4	8	4	58	68	0
25	7	0	22*	0	10	2	8	-4	49	39	4	4	8	5	-11*	0	13
25	7	1	-23*	0	9	2	8	-3	65	60	6	4	8	6	-20*	0	17
25	7	2	7*	0	18	2	8	-2	26*	0	5	5	8	7	12*	0	23
26	7	-2	-37*	0	12	2	8	-1	28*	0	6	5	8	8	22*	0	22
26	7	-1	22*	0	10	2	8	0	60	70	3	5	8	-7	0*	0	11
26	7	0	12*	0	15	2	8	1	110	108	4	5	8	-6	-32*	0	22
26	7	1	-7*	0	25	2	8	2	53	46	4	5	8	-5	46	41	4
0	8	0	103	111	4	2	8	3	50	57	4	5	8	-4	-22*	0	12
0	8	1	63	72	5	2	8	4	78	78	3	5	8	-3	-15*	0	14
0	8	2	82	77	9	2	8	5	135	137	4	5	8	-2	122	122	6
0	8	3	59	40	3	2	8	6	19*	0	15	5	8	-1	30*	0	20
0	8	4	51	40	4	2	8	7	26*	0	9	5	8	0	-7*	0	45
0	8	5	28*	0	6	2	8	8	29*	0	9	5	8	1	62	45	3

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
8	8	1	133	139	4	11	8	-4	93	90	4	14	8	-3	16*	0	18
8	8	0	55	43	3	11	8	-3	150	142	4	14	8	-2	58	57	4
8	8	1	159	165	4	11	8	-2	41	30	5	14	8	-1	-14*	0	15
8	8	2	121	130	4	11	8	-1	51	46	4	14	8	0	-5*	0	14
8	8	3	59	52	3	11	8	0	95	91	4	14	8	1	39	40	5
8	8	4	7*	0	22	11	8	1	18*	0	14	14	8	2	7*	0	21
8	8	5	-9*	0	19	11	8	2	-22*	0	12	14	8	3	43	42	5
8	8	6	-25*	0	8	11	8	3	35	31	5	14	8	4	10*	0	22
8	8	7	-19*	0	10	11	8	4	19*	0	9	14	8	5	41	33	6
8	8	8	-11*	0	14	11	8	5	42	38	5	14	8	6	19*	0	11
9	8	-8	0*	0	33	11	8	6	8*	0	25	14	8	7	-21*	0	16
9	8	-7	-41*	0	11	11	8	7	-26*	0	13	15	8	-6	15*	0	21
9	8	-6	23*	0	9	12	8	-8	24*	0	10	15	8	-5	16*	0	20
9	8	-5	36*	0	6	12	8	-7	-23*	0	17	15	8	-4	-25*	0	15
9	8	-4	46	28	4	12	8	-6	22*	0	16	15	8	-3	71	68	4
9	8	-3	114	118	4	12	8	-5	-18*	0	17	15	8	-2	-18*	0	14
9	8	-2	175	181	4	12	8	-4	58	56	4	15	8	-1	34*	0	6
9	8	-1	117	111	4	12	8	-3	61	55	4	15	8	0	38	31	5
9	8	0	-5*	0	21	12	8	-2	9*	0	19	15	8	1	-13*	0	10
9	8	1	115	119	4	12	8	-1	122	119	4	15	8	2	63	57	4
9	8	2	65	83	3	12	8	0	11*	0	17	15	8	3	16*	0	13
9	8	3	72	82	3	12	8	1	67	57	3	15	8	4	-28*	0	14
9	8	4	45	41	5	12	8	2	-8*	0	18	15	8	5	-11*	0	9
9	8	5	-21*	0	14	12	8	3	-34*	0	17	15	8	6	26*	0	23
9	8	6	-26*	0	7	12	8	4	12*	0	17	15	8	7	-13*	0	14
9	8	7	-18*	0	17	12	8	5	-17*	0	13	16	8	-6	27*	0	10
9	8	8	-23*	0	15	12	8	6	-43*	0	9	16	8	-5	37*	0	10
10	8	-8	-39*	0	11	12	8	7	21*	0	17	16	8	-4	-14*	0	21
10	8	-7	-15*	0	12	13	8	-8	-33*	0	13	16	8	-3	29*	0	6
10	8	-6	22*	0	9	13	8	-7	41*	0	6	16	8	-2	-21*	0	27
10	8	-5	51	43	5	13	8	-6	51	40	5	16	8	-1	36	23	5
10	8	-4	73	66	3	13	8	-5	45	44	6	16	8	0	-10*	0	19
10	8	-3	50	33	4	13	8	-4	39	17	6	16	8	1	-22*	0	20
10	8	-2	81	79	3	13	8	-3	-22*	0	13	16	8	2	32*	0	7
10	8	-1	90	94	4	13	8	-2	15*	0	12	16	8	3	17*	0	9
10	8	0	44	42	4	13	8	-1	-25*	0	9	16	8	4	-19*	0	28
10	8	1	58	51	3	13	8	0	-32*	0	8	16	8	5	32*	0	31
10	8	2	25*	0	6	13	8	1	37	36	5	16	8	6	0*	0	14
10	8	3	30*	0	7	13	8	2	83	77	4	16	8	7	-7*	0	24
10	8	4	34*	0	6	13	8	3	40	38	5	16	8	8	20*	0	17
10	8	5	20*	0	10	13	8	4	-21*	0	13	17	8	-7	17*	0	20
10	8	6	22*	0	10	13	8	5	45	38	5	17	8	-6	-12*	0	18
10	8	7	-21*	0	15	13	8	6	-47*	0	9	17	8	-5	20*	0	9
11	8	-8	-4*	0	20	14	8	-7	-15*	0	20	17	8	-4	-9*	0	20
11	8	-7	-18*	0	17	14	8	-6	30*	0	9	17	8	-3	21*	0	17
11	8	-6	-12*	0	20	14	8	-5	79	72	5	17	8	-2	-24*	0	11
11	8	-5	54	53	5	14	8	-4	16*	0	17	17	8	-1	0	0	20

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
21	8	0	24*	0	9	1	9	-7	34*	0	8	3	9	7	-22*	0	9	6	9	4	28*	0	7
21	8	1	32*	0	8	1	9	-6	-10*	0	13	3	9	8	-33*	0	12	6	9	5	30*	0	6
21	8	2	49*	35	5	1	9	-5	40	41	6	4	9	-8	-20*	0	11	6	9	6	13*	0	13
21	8	3	17*	0	19	1	9	-4	41	40	5	4	9	-7	40*	0	16	6	9	7	-23*	0	15
21	8	4	19*	0	17	1	9	-3	20*	0	8	4	9	-6	-24*	0	14	6	9	8	-27*	0	14
22	8	-5	-14*	0	19	1	9	-2	88	85	4	4	9	-5	34*	0	17	7	9	-8	-41*	0	11
22	8	-4	-17*	0	17	1	9	-1	-18*	0	7	4	9	-4	21*	0	8	7	9	-7	-12*	0	13
22	8	-3	-13*	0	19	1	9	0	8*	0	16	4	9	-3	19*	0	8	7	9	-6	-19*	0	16
22	8	-2	-25*	0	14	1	9	1	25*	0	6	4	9	-2	23*	0	6	7	9	-5	7*	0	22
22	8	-1	-21*	0	16	1	9	2	0*	0	24	4	9	-1	45	44	4	7	9	-4	28*	0	7
22	8	0	-21*	0	16	1	9	3	25*	0	7	4	9	0	-17*	0	7	7	9	-3	32*	0	6
22	8	1	-21*	0	16	1	9	4	16*	0	10	4	9	1	27*	0	6	7	9	-2	-10*	0	17
22	8	2	-15*	0	18	1	9	5	55	56	0	4	9	2	59	69	3	7	9	-1	-2*	0	16
22	8	3	-39*	0	7	1	9	6	4*	0	18	4	9	3	34	34	5	7	9	0	84	96	4
22	8	4	-18*	0	17	1	9	7	-43*	0	10	4	9	4	47	56	4	7	9	1	0*	0	25
23	8	-4	12*	0	20	1	9	8	29*	0	8	4	9	5	25*	0	10	7	9	2	37	37	4
23	8	-3	-36*	0	12	1	9	-8	8*	0	25	4	9	6	-18*	0	9	7	9	3	-17*	0	8
23	8	-2	24*	0	10	1	9	-7	0*	0	33	4	9	7	22*	0	9	7	9	4	-22*	0	13
23	8	-1	-33*	0	7	2	9	-6	-23*	0	15	5	9	8	28*	0	25	7	9	5	7*	0	24
23	8	0	-22*	0	16	2	9	-5	51	54	5	5	9	-8	8*	0	25	7	9	6	22*	0	9
23	8	1	-19*	0	10	2	9	-4	-22*	0	8	5	9	-7	20*	0	10	7	9	7	20*	0	16
23	8	2	-29*	0	13	2	9	-3	46	49	4	5	9	-6	17*	0	11	7	9	8	-24*	0	15
23	8	3	-41*	0	11	2	9	-2	37	35	4	5	9	-5	19*	0	9	8	9	-8	26*	0	9
24	8	-3	-41*	0	11	2	9	-1	-15*	0	8	5	9	-4	27*	0	6	8	9	-7	18*	0	18
24	8	-2	0*	0	31	2	9	0	83	90	3	5	9	-3	37	32	5	8	9	-6	4*	0	18
24	8	-1	42*	0	6	2	9	1	5*	0	14	5	9	-2	16*	0	9	8	9	-5	23*	0	9
24	8	0	45*	28	6	2	9	2	-31*	0	9	5	9	-1	42	48	4	8	9	-4	22*	0	8
24	8	1	-29*	0	13	2	9	3	12*	0	11	5	9	0	13*	0	10	8	9	-3	76	71	3
24	8	2	-12*	0	14	2	9	4	23*	0	8	5	9	1	46	49	4	8	9	-2	20*	93	8
25	8	-2	-40*	0	11	2	9	5	-13*	0	17	5	9	2	44	59	4	8	9	-1	89	93	4
25	8	-1	15*	0	21	2	9	6	-14*	0	10	5	9	3	13*	0	16	8	9	0	0*	0	19
25	8	0	17*	0	12	2	9	7	-19*	0	17	5	9	4	23*	0	22	8	9	1	-22*	0	12
25	8	1	23*	0	17	2	9	8	-7*	0	25	5	9	5	7*	0	22	8	9	2	42	51	4
0	9	9	-15*	0	10	3	9	-8	-21*	0	17	5	9	6	-23*	0	14	8	9	3	-7*	0	12
0	9	9	35	40	5	3	9	-7	-12*	0	21	5	9	7	25*	0	18	8	9	4	16*	0	16
0	9	9	39	35	5	3	9	-6	-50*	0	9	5	9	8	-27*	0	13	8	9	5	-29*	0	11
0	9	9	23*	0	7	3	9	-5	25*	0	8	6	9	9	-33*	0	13	8	9	6	-10*	0	21
0	9	9	87	77	3	3	9	-4	42	41	5	6	9	-8	31*	0	8	8	9	7	-7*	0	24
0	9	9	67	77	3	3	9	-3	-23*	0	11	6	9	-6	29*	0	8	8	9	8	15*	0	21
0	9	9	45	40	5	3	9	-2	6*	0	20	6	9	-5	-19*	0	9	9	9	-8	-16*	0	12
0	9	9	15*	0	12	3	9	-1	74	82	4	6	9	-4	34*	0	6	9	9	-7	-43*	0	10
0	9	9	0*	0	29	3	9	0	10*	0	17	6	9	-3	57	50	6	9	9	-6	0*	0	30
0	9	9	0	0	23	3	9	1	101	120	3	6	9	-2	64	76	3	9	9	-5	-27*	0	13
0	9	9	-12*	0	12	3	9	2	77	86	4	6	9	-1	71	97	4	9	9	-4	16*	0	11
0	9	9	-7*	0	24	3	9	3	12*	0	18	6	9	0	90	0	3	9	9	-3	19*	0	15
0	9	9	15*	0	13	3	9	4	-23*	0	13	6	9	1	0*	0	4	9	9	-2	52	51	4
1	9	-8	36*	0	7	3	9	5	-23*	0	13	6	9	2	-17*	0	12	9	9	-1	55	57	4

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
9	9	1	-10*	0	17	12	9	3	18*	0	9	16	9	-6	-18*	0	11
9	9	2	-26*	0	11	12	9	4	34*	0	6	16	9	-5	-15*	0	18
9	9	3	41	41	5	12	9	5	-21*	0	16	16	9	-4	-29*	0	13
9	9	4	45	51	5	12	9	6	-19*	0	10	16	9	-3	11*	0	22
9	9	5	-8*	0	14	12	9	7	-11*	0	14	16	9	-2	39	37	6
9	9	6	-3*	0	18	13	9	-7	15*	0	22	16	9	-1	-20*	0	14
9	9	7	12*	0	21	13	9	-6	-13*	0	20	16	9	0	28*	0	7
10	9	-8	-31*	0	14	13	9	-5	42	40	6	16	9	1	-21*	0	8
10	9	-7	-17*	0	18	13	9	-4	47	52	5	16	9	2	64	49	4
10	9	-6	14*	0	19	13	9	-3	38	38	6	16	9	3	39	24	6
10	9	-5	-15*	0	12	13	9	-2	32*	0	6	16	9	4	0*	0	31
10	9	-4	12*	0	17	13	9	-1	32*	0	6	16	9	5	55*	49	5
10	9	-3	80	80	3	13	9	0	-20*	0	7	16	9	6	-18*	0	19
10	9	-2	76	69	3	13	9	1	0*	0	12	17	9	-6	-28*	0	15
10	9	-1	27*	48	4	13	9	2	39	0	25	17	9	-5	-24*	0	15
10	9	0	-30*	0	10	13	9	3	-9*	0	13	17	9	-4	-10*	0	20
10	9	1	-8*	0	18	13	9	4	26*	0	8	17	9	-3	-24*	0	8
10	9	2	38	38	5	13	9	5	-25*	0	15	17	9	-2	0*	0	29
10	9	3	19*	0	14	13	9	6	27*	0	9	17	9	-1	32*	0	6
10	9	4	17*	0	16	14	9	-7	-12*	0	14	17	9	0	-10*	0	13
10	9	5	-21*	0	14	14	9	-6	-21*	0	10	17	9	1	13*	0	18
10	9	6	-29*	0	13	14	9	-5	-18*	0	17	17	9	2	14*	0	12
11	9	-7	-42*	0	11	14	9	-4	-6*	0	23	17	9	3	0*	0	31
11	9	-6	-39*	0	11	14	9	-3	-12*	0	11	17	9	4	-7*	0	17
11	9	-5	29*	0	8	14	9	-2	62	54	4	18	9	5	-7*	0	24
11	9	-4	26*	0	8	14	9	-1	29*	0	7	18	9	-6	-28*	0	24
11	9	-3	47	48	5	14	9	0	-33*	0	10	18	9	-5	20*	0	14
11	9	-2	10*	42	20	14	9	1	24*	0	7	18	9	-4	-31*	0	17
11	9	-1	39	42	5	14	9	2	10*	0	19	18	9	-3	-3*	0	18
11	9	0	46	54	4	14	9	3	-20*	0	15	18	9	-2	-22*	0	8
11	9	1	21*	0	7	14	9	4	-22*	0	14	18	9	-1	-26*	0	12
11	9	2	16*	0	15	14	9	5	-42*	0	11	18	9	0	31*	0	6
11	9	3	30*	0	8	15	9	-6	23*	0	25	18	9	1	14*	0	7
11	9	4	27*	0	10	15	9	-5	-33*	0	12	18	9	2	-39*	0	21
11	9	5	-14*	0	12	15	9	-4	-33*	0	12	18	9	3	9*	0	16
11	9	6	-14*	0	8	15	9	-3	31*	0	19	19	9	4	-30*	0	11
11	9	7	32*	0	15	15	9	-2	-9*	0	19	19	9	5	-5*	0	16
12	9	-7	20*	0	15	15	9	-1	-29*	0	19	19	9	-6	-20*	0	15
12	9	-6	34*	0	7	15	9	0	48	43	4	19	9	-5	53	24	4
12	9	-5	19*	0	10	15	9	1	-20*	0	8	19	9	-4	-22*	0	14
12	9	-4	14*	0	18	15	9	2	18*	0	17	19	9	-3	49	31	4
12	9	-3	30*	0	20	15	9	3	19*	0	16	19	9	-2	26*	0	8
12	9	-2	-8*	0	10	15	9	4	16*	0	18	19	9	-1	-7*	0	16
12	9	-1	-32*	0	8	15	9	5	-29*	0	18	19	9	0	54*	52	6
12	9	0	19*	51	8	15	9	6	-4*	0	19	19	9	1	-11*	0	21
12	9	1	51	51	4	15	9	7		0	19	19	9	2	-23*	0	17

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
0	10	7	-41*	0	11	3	10	2	-16*	0	13	6	10	3	16*	0	15
0	10	7	-19*	0	15	3	10	3	17*	0	15	6	10	4	-16*	0	9
0	10	8	-32*	0	12	3	10	4	19*	0	14	6	10	5	11*	0	21
0	10	8	5*	0	19	3	10	5	-22*	0	13	6	10	6	-40*	0	11
1	10	-8	-7*	0	25	3	10	6	-16*	0	17	6	10	7	-23*	0	9
1	10	-7	-10*	0	22	3	10	7	-19*	0	17	7	10	-7	-38*	0	12
1	10	-6	8*	0	22	4	10	-8	19*	0	17	7	10	-6	21*	0	10
1	10	-5	30*	0	7	4	10	-7	-29*	0	13	7	10	-5	25*	0	18
1	10	-4	73	69	3	4	10	-6	48	38	5	7	10	-4	-18*	0	14
1	10	-3	28*	0	6	4	10	-5	7*	0	24	7	10	-3	32*	0	6
1	10	-2	54	57	4	4	10	-4	55	58	4	7	10	-2	-25*	0	12
1	10	-1	-17*	0	13	4	10	-3	45	39	4	7	10	-1	-8*	0	18
1	10	0	59	67	3	4	10	-2	43	15	4	7	10	0	-22*	0	12
1	10	1	60	71	4	4	10	-1	53	52	4	7	10	1	36	44	5
1	10	2	92	114	4	4	10	0	85	88	3	7	10	2	17*	0	15
1	10	3	48	45	4	4	10	1	-10*	0	11	7	10	3	-6*	0	21
1	10	4	31*	0	6	4	10	2	15*	0	10	7	10	4	19*	0	9
1	10	5	-23*	0	8	4	10	3	50	49	4	7	10	5	-19*	0	6
1	10	6	-11*	0	13	4	10	4	15*	0	10	7	10	6	34*	0	17
1	10	7	29*	0	8	4	10	5	18*	0	15	7	10	7	21*	0	13
1	10	8	-32*	0	13	4	10	6	19*	0	16	8	10	-7	-32*	0	9
2	10	-8	-26*	0	9	4	10	7	0*	0	30	8	10	-6	-20*	0	16
2	10	-7	-30*	0	12	5	10	-8	23*	0	25	8	10	-5	20*	0	7
2	10	-6	15*	0	12	5	10	-7	-19*	0	17	8	10	-4	26*	0	8
2	10	-5	42	33	6	5	10	-6	15*	0	12	8	10	-3	15*	0	10
2	10	-4	58	58	4	5	10	-5	45	39	5	8	10	-2	38	39	5
2	10	-3	-27*	0	12	5	10	-4	-30*	0	10	8	10	-1	-22*	0	12
2	10	-2	74	76	3	5	10	-3	42	46	4	8	10	0	95	96	4
2	10	-1	33*	0	5	5	10	-2	49	49	4	8	10	1	-12*	0	10
2	10	0	22*	0	7	5	10	-1	11*	0	17	8	10	2	19*	0	14
2	10	1	19*	0	8	5	10	0	74	90	3	8	10	3	16*	0	16
2	10	2	37	44	5	5	10	1	12*	0	11	8	10	4	-10*	0	9
2	10	3	71	86	3	5	10	2	36	32	5	8	10	5	20*	0	14
2	10	4	12*	0	12	5	10	3	16*	0	16	8	10	6	-21*	0	10
2	10	5	-13*	0	18	5	10	4	-6*	0	23	9	10	-7	14*	0	18
2	10	6	-13*	0	14	5	10	5	-18*	0	15	9	10	-6	-36*	0	12
2	10	7	-29*	0	17	5	10	6	20*	0	11	9	10	-5	-15*	0	7
2	10	8	19*	0	13	6	10	-7	-15*	0	12	9	10	-4	32*	0	10
3	10	-8	-14*	0	19	6	10	-6	7*	0	23	9	10	-3	-15*	0	18
3	10	-7	18*	0	24	6	10	-5	-19*	0	15	9	10	-2	37*	0	6
3	10	-6	-6*	0	22	6	10	-4	24*	0	18	12	10	0	22*	55	8
3	10	-5	23*	0	6	6	10	-3	83	84	3	12	10	1	17*	0	10
3	10	-4	31*	0	6	6	10	-2	83	27	5	12	10	2	15*	0	18
3	10	-3	60	58	3	6	10	-1	33	84	3	12	10	3	-25*	0	12
3	10	-2	14*	0	15	6	10	0	17*	0	13	12	10	4	-13*	0	18
3	10	-1	92	108	4	6	10	1	45	51	4	13	10	5	-11*	0	22
3	10	0	16*	0	14	6	10	2	-6*	0	19	13	10	6	-24*	0	9
3	10	1				6	10	3		0		13	10	7	-20*	0	15

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
13	10	-3	-21*	0	9	17	10	-4	-33*	0	11	23	10	-1	-26*	0	15	3	11	-3	17*	0	9
13	10	-2	15*	0	18	17	10	-3	-31*	0	12	23	10	0	-34*	0	13	3	11	-2	-18*	0	14
13	10	-1	-6*	0	15	17	10	-2	16*	0	11	0	11	1	-3*	0	23	3	11	-1	-19*	0	13
13	10	0	30*	0	7	17	10	-1	31*	0	7	0	11	2	-4*	0	23	3	11	0	0*	0	27
13	10	1	32*	0	6	17	10	0	35*	0	7	0	11	3	21*	0	8	3	11	1	-18*	0	8
13	10	2	26*	0	7	17	10	1	33*	0	7	0	11	3	-27*	0	11	3	11	2	42	40	5
13	10	3	52	36	4	17	10	2	11*	0	21	0	11	3	-27*	0	11	3	11	2	42	40	5
13	10	4	-16*	0	11	17	10	3	-17*	0	16	0	11	4	37*	0	6	3	11	3	-34*	0	10
13	10	5	22*	0	17	17	10	4	17*	0	18	0	11	4	30*	0	7	3	11	4	-30*	0	12
13	10	6	20*	0	11	17	10	5	14*	0	21	0	11	5	-14*	0	17	3	11	5	17*	0	15
14	10	-6	18*	0	12	17	10	-5	-14*	0	23	0	11	5	-14*	0	8	3	11	6	-41*	0	10
14	10	-5	22*	0	16	18	10	-4	-19*	0	17	0	11	6	-17*	0	15	3	11	7	-18*	0	18
14	10	-4	14*	0	13	18	10	-3	-42*	0	12	0	11	6	-28*	0	9	4	11	-7	-24*	0	9
14	10	-3	26*	0	8	18	10	-2	-13*	0	11	0	11	7	17*	0	11	4	11	-6	-10*	0	8
14	10	-2	0*	0	28	18	10	-1	-18*	0	16	1	11	7	-21*	0	16	4	11	-5	-10*	0	19
14	10	-1	-13*	0	11	18	10	0	-12*	0	21	1	11	-6	-18*	0	11	4	11	-4	13*	0	18
14	10	0	-11*	0	17	18	10	1	11*	0	21	1	11	-5	-25*	0	13	4	11	-3	16*	0	10
14	10	1	21*	0	8	18	10	2	6*	0	17	1	11	-4	-34*	0	11	4	11	-2	36	17	5
14	10	2	32*	0	7	18	10	3	39*	0	7	1	11	-3	24*	0	8	4	11	0	-27*	0	11
14	10	3	21*	0	9	18	10	4	5*	0	19	1	11	-2	42	32	5	4	11	1	20*	0	11
14	10	4	-3*	0	18	19	10	-4	17*	0	12	1	11	-1	-9*	0	12	4	11	2	47	62	5
14	10	5	19*	0	11	19	10	-3	-23*	0	15	1	11	0	10*	0	12	4	11	3	-24*	0	13
15	10	-6	12*	0	23	19	10	-2	46*	30	5	1	11	1	22*	0	8	4	11	4	-16*	0	10
15	10	-5	-30*	0	8	19	10	-1	-18*	0	10	1	11	2	26*	0	6	4	11	5	14*	0	11
15	10	-4	-22*	0	16	19	10	0	-13*	0	21	1	11	3	14*	0	17	4	11	6	-13*	0	19
15	10	-3	37*	0	15	19	10	1	-11*	0	14	1	11	4	20*	0	15	5	11	7	-35*	0	12
15	10	-2	-22*	0	6	19	10	2	20*	0	17	1	11	5	-20*	0	10	5	11	-7	22*	0	16
15	10	-1	-15*	0	15	19	10	3	-35*	0	11	1	11	6	-41*	0	10	5	11	-6	22*	0	15
15	10	0	-22*	0	17	19	10	4	-28*	0	14	1	11	7	-13*	0	17	5	11	-5	10*	0	17
15	10	1	21*	0	9	20	10	-4	-7*	0	23	2	11	-7	-24*	0	13	5	11	-4	30*	0	21
15	10	2	-9*	0	19	20	10	-3	0*	0	31	2	11	-6	-15*	0	11	5	11	-3	10*	0	6
15	10	3	23*	0	8	20	10	-2	-13*	0	19	2	11	-5	-24*	0	12	5	11	-2	27*	0	7
15	10	4	-17*	0	10	20	10	-1	19*	0	11	2	11	-4	-14*	0	8	5	11	-1	13*	0	11
15	10	5	8*	0	18	20	10	0	-17*	0	11	2	11	-3	-19*	0	5	5	11	0	27*	0	6
16	10	-6	-18*	0	24	20	10	1	-20*	0	15	2	11	-2	36	38	12	5	11	1	10*	0	19
16	10	-5	21*	0	18	20	10	2	-9*	0	17	2	11	-1	-20*	0	12	5	11	2	36*	0	15
16	10	-4	-20*	0	10	20	10	3	19*	0	18	2	11	0	47	53	5	5	11	3	24*	0	8
16	10	-3	-45*	0	18	21	10	-3	-27*	0	8	2	11	1	33*	0	15	5	11	4	13*	0	12
16	10	-2	-14*	0	10	21	10	-2	27*	0	8	2	11	2	-16*	0	16	5	11	5	20*	0	11
16	10	-1	-26*	0	18	21	10	-1	21*	0	14	2	11	3	16*	0	14	5	11	6	16*	0	13
16	10	0	37*	0	6	21	10	0	11*	0	12	2	11	4	-10*	0	20	6	11	7	-14*	0	19
16	10	1	18*	0	10	21	10	1	19*	0	11	2	11	5	-25*	0	8	6	11	-6	-37*	0	11
16	10	2	-10*	0	12	22	10	-2	21*	0	18	3	11	6	-22*	0	9	6	11	-5	24*	0	9
16	10	3	14*	0	11	22	10	-1	-18*	0	17	3	11	-7	-21*	0	17	6	11	-4	17*	0	16
16	10	4	-20*	0	15	22	10	0	-30*	0	12	3	11	-6	-25*	0	30	6	11	-3	-11*	0	18
16	10	5	-32*	0	13	22	10	1	17*	0	12	3	11	-5	-10*	0	8	6	11	-2	-24*	0	12
17	10	-5	-35*	0	12	22	10	2	-29*	0	14	3	11	-4	10*	0	20	6	11	-1	18*	0	9

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
6	11	0	7*	0	21	9	11	6	15*	0	13	13	11	3	-29*	0	12	18	11	0	28*	0	9
6	11	1	37	32	5	10	11	-6	17*	0	12	13	11	4	22*	0	19	18	11	1	18*	0	11
6	11	2	37	47	6	10	11	-5	-10*	0	21	13	11	5	5*	0	19	18	11	2	-17*	0	17
6	11	3	-22*	0	12	10	11	-4	-29*	0	13	14	11	-5	-22*	0	15	18	11	3	-23*	0	16
6	11	4	-14*	0	17	10	11	-3	11*	0	21	14	11	-4	-15*	0	12	19	11	-3	15*	0	13
6	11	5	-35*	0	11	10	11	-2	37*	0	6	14	11	-3	-16*	0	18	19	11	-2	-32*	0	13
6	11	6	14*	0	21	10	11	-1	-30*	0	11	14	11	-2	45	36	6	19	11	-1	0*	0	31
6	11	7	-18*	0	18	10	11	0	18*	0	11	14	11	-1	13*	0	20	19	11	0	-29*	0	19
7	11	-7	-36*	0	12	10	11	1	29*	0	7	14	11	0	-12*	0	20	19	11	1	-15*	0	13
7	11	-6	13*	0	13	10	11	2	22*	0	9	14	11	1	27*	0	8	19	11	2	-25*	0	14
7	11	-5	26*	0	8	10	11	3	39	32	6	14	11	2	-33*	0	12	19	11	3	-16*	0	17
7	11	-4	-25*	0	13	10	11	4	-31*	0	12	14	11	3	28*	0	18	20	11	-2	32*	0	8
7	11	-3	34*	0	16	10	11	5	-25*	0	9	14	11	4	-17*	0	18	20	11	-1	-23*	0	16
7	11	-2	14*	0	11	10	11	6	-13*	0	12	14	11	5	-25*	0	9	20	11	0	-31*	0	12
7	11	-1	33*	0	6	11	11	-6	-37*	0	13	15	11	-5	-16*	0	18	20	11	1	16*	0	17
7	11	0	60	59	4	11	11	-5	21*	0	10	15	11	-4	-19*	0	14	21	11	-1	21*	0	15
7	11	1	-17*	0	14	11	11	-4	-33*	0	12	15	11	-3	-29*	0	16	21	11	0	-23*	0	11
7	11	2	-11*	0	12	11	11	-3	-17*	0	18	15	11	-2	40*	0	20	21	11	1	-17*	0	18
7	11	3	-11*	0	13	11	11	-2	20*	0	9	15	11	-1	-10*	0	20	21	11	2	12*	0	14
7	11	4	-23*	0	20	11	11	-1	21*	0	9	15	11	0	56	44	4	0	12	1	-20*	0	13
7	11	5	16*	0	13	11	11	0	-6*	0	22	15	11	1	1	0	19	0	12	2	23*	0	17
7	11	6	-34*	0	12	11	11	1	-14*	0	11	15	11	2	0*	0	31	0	12	3	-15*	0	10
8	11	-7	-27*	0	14	11	11	2	46	53	6	15	11	3	-23*	0	9	0	12	4	-26*	0	7
8	11	-6	-13*	0	13	11	11	3	-17*	0	10	15	11	4	-21*	0	17	0	12	5	0*	0	30
8	11	-5	-26*	0	14	11	11	4	-10*	0	21	15	11	5	-29*	0	13	0	12	6	-18*	0	16
8	11	-4	27*	0	8	11	11	5	19*	0	17	16	11	-5	-33*	0	14	0	12	7	-13*	0	18
8	11	-3	-18*	0	10	11	11	-6	-28*	0	30	16	11	-4	-42*	0	11	0	12	8	2*	0	15
8	11	-2	10*	0	10	12	11	-5	5*	0	19	16	11	-3	21*	0	10	0	12	9	8*	0	20
8	11	-1	19*	0	21	12	11	-4	-25*	0	13	16	11	-2	18*	0	11	0	12	10	-13*	0	14
8	11	0	-15*	0	9	12	11	-3	-18*	0	16	16	11	-1	16*	0	14	1	12	11	-14*	0	21
8	11	1	-14*	0	10	12	11	-2	-30*	0	11	16	11	0	-21*	0	10	1	12	12	-25*	0	13
8	11	2	-41*	0	10	12	11	-1	13*	0	18	16	11	1	20*	0	15	1	12	13	-9*	0	20
8	11	3	41	46	6	12	11	0	-12*	0	19	16	11	2	-24*	0	14	1	12	14	20*	0	15
8	11	4	-20*	0	16	12	11	1	0*	0	31	16	11	3	29*	0	15	1	12	15	-16*	0	15
8	11	5	15*	0	21	12	11	2	32*	0	7	17	11	-4	-23*	0	13	1	12	16	-15*	0	10
9	11	-6	-57*	0	9	12	11	3	11*	0	22	17	11	-3	-28*	0	15	1	12	17	-5*	0	10
9	11	-5	-17*	0	17	12	11	4	-21*	0	16	17	11	-2	-25*	0	14	1	12	18	-4*	0	17
9	11	-4	-40*	0	10	12	11	5	-27*	0	14	17	11	-1	-21*	0	15	1	12	19	-11*	0	13
9	11	-3	-28*	0	11	13	11	-6	-11*	0	22	17	11	0	-23*	0	17	1	12	20	-26*	0	12
9	11	-2	-18*	0	14	13	11	-5	-26*	0	13	17	11	1	8*	0	24	1	12	21	-33*	0	18
9	11	-1	29*	0	5	13	11	-4	-15*	0	11	17	11	2	-23*	0	25	1	12	22	-29*	0	13
9	11	0	47	45	9	13	11	-3	21*	0	10	17	11	3	21*	0	17	1	12	23	23*	0	9
9	11	1	-38*	0	9	13	11	-2	-6*	0	22	18	11	4	-14*	0	21	1	12	24	30*	0	7
9	11	2	-16*	0	10	13	11	-1	46	37	5	18	11	-3	-27*	0	19	1	12	25	33*	0	15
9	11	3	22*	0	9	13	11	0	39	21	6	18	11	-2	32*	0	8	1	12	26	-19*	0	15
9	11	4	-16*	0	17	13	11	1	-12*	0	20	18	11	-1	-20*	0	10	1	12	27	-23*	0	13
9	11	5	16*	0	18	13	11	2	-12*	0	20	18	11	1	-20*	0	10	1	12	28	-23*	0	13

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	12	0	-15*	0	16	6	12	-4	-7*	0	22	10	12	-5	-22*	0	15
2	12	1	-6*	0	21	6	12	-3	-10*	0	21	10	12	-4	-10*	0	22
2	12	2	7*	0	16	6	12	-2	-20*	0	14	10	12	-3	-39*	0	10
2	12	3	-26*	0	13	6	12	-1	-22*	0	13	10	12	-2	13*	0	13
2	12	4	20*	0	10	6	12	0	-13*	0	17	10	12	-1	-22*	0	15
2	12	5	-20*	0	16	6	12	1	-17*	0	16	10	12	0	28*	0	7
2	12	6	19*	0	18	6	12	2	17*	0	11	10	12	1	13*	0	20
3	12	-6	-17*	0	18	6	12	3	-24*	0	8	10	12	2	34*	0	7
3	12	-5	-15*	0	18	6	12	4	30*	0	8	10	12	3	30*	0	22
3	12	-4	-37*	0	10	6	12	5	35*	0	7	10	12	4	24*	0	20
3	12	-3	-14*	0	18	6	12	6	12*	0	15	10	12	5	-22*	0	14
3	12	-2	-12*	0	18	6	12	-6	9*	0	25	11	12	-5	-21*	0	12
3	12	-1	19*	0	14	7	12	-5	-19*	0	17	11	12	-4	14*	0	17
3	12	0	-13*	0	17	7	12	-4	-22*	0	14	11	12	-3	16*	0	10
3	12	1	-11*	0	18	7	12	-3	-34*	0	11	11	12	-2	-10*	0	15
3	12	2	0*	0	30	7	12	-2	-7*	0	14	11	12	-1	-35*	0	14
3	12	3	17*	0	17	7	12	-1	-12*	0	18	11	12	0	10*	0	16
3	12	4	-8*	0	24	7	12	0	-28*	0	11	11	12	1	15	0	17
3	12	5	-18*	0	15	7	12	1	-12*	0	12	11	12	2	39*	0	17
3	12	6	-31*	0	13	7	12	2	-21*	0	14	11	12	3	14*	0	8
4	12	-6	-21*	0	16	7	12	3	40*	0	6	11	12	4	-25*	0	13
4	12	-5	32*	0	13	7	12	4	-9*	0	15	11	12	5	-34*	0	14
4	12	-4	-30*	0	15	7	12	5	-14*	0	21	12	12	-5	17*	0	25
4	12	-3	20*	0	15	8	12	-6	-17*	0	16	12	12	-4	-42*	0	17
4	12	-2	-28*	0	15	8	12	-5	-30*	0	12	12	12	-3	-33*	0	11
4	12	-1	-20*	0	10	8	12	-4	-17*	0	11	12	12	-2	-29*	0	14
4	12	0	18*	0	17	8	12	-3	-22*	0	15	12	12	-1	20*	0	12
4	12	1	-16*	0	20	8	12	-2	-15*	0	16	12	12	0	-11*	0	8
4	12	2	14*	0	31	8	12	-1	50	42	5	12	12	1	-20*	0	17
4	12	3	0*	0	16	8	12	0	39	34	6	12	12	2	-21*	0	13
4	12	4	-19*	0	19	8	12	1	29*	0	17	13	12	3	13*	0	15
5	12	-6	16*	0	19	8	12	2	-15*	0	19	13	12	4	-24*	0	14
5	12	-5	14*	0	19	8	12	3	-36*	0	22	13	12	5	26*	0	23
5	12	-4	-21*	0	17	9	12	-6	-21*	0	15	13	12	-3	-22*	0	22
5	12	-3	15*	0	14	9	12	-5	-25*	0	12	13	12	-2	19*	0	17
5	12	-2	19*	0	12	9	12	-4	-9*	0	8	13	12	-1	-12*	0	14
5	12	-1	-28*	0	12	9	12	-3	14*	0	15	13	12	0	-27*	0	11
5	12	0	44	39	5	9	12	-2	-26*	0	13	13	12	1	27*	0	13
5	12	1	-6*	0	15	9	12	-1	0*	0	29	14	12	2	-23*	0	18
5	12	2	-35*	0	11	9	12	0	44	45	5	14	12	3	17*	0	19
5	12	3	-24*	0	14	9	12	1	37*	0	7	14	12	4	-28*	0	15
5	12	4	-27*	0	13	9	12	2	22*	0	17	14	12	-2	-10*	0	12
5	12	5	-22*	0	10	9	12	3	-40*	0	11	14	12	-1	19*	0	11
6	12	-6	12*	0	20	9	12	4				14	12	0			21
6	12	-5				9	12	5				14	12	1			

Reflections flagged with an asterisk were considered unobserved.

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
1	13	3	-7*	0	23	6	13	-4	12*	0	21	10	13	3	17*	0	16
1	13	4	36*	0	6	6	13	-3	-17*	0	18	10	13	4	17*	0	12
1	13	5	-18*	0	17	6	13	-2	-14*	0	18	11	13	-4	27*	0	9
2	13	-5	-13*	0	21	6	13	-1	-28*	0	14	11	13	-3	16*	0	13
2	13	-4	-7*	0	16	6	13	0	10*	0	14	11	13	-2	-19*	0	11
2	13	-3	24*	0	9	6	13	1	-5*	0	17	11	13	-1	8*	0	25
2	13	-2	-24*	0	14	6	13	2	25*	0	8	11	13	0	20*	0	17
2	13	-1	-20*	0	21	6	13	3	-29*	0	12	11	13	1	14*	0	20
2	13	0	-21*	0	14	6	13	4	-20*	0	10	11	13	2	-32*	0	12
2	13	1	-40*	0	10	6	13	5	-33*	0	12	11	13	3	19*	0	16
2	13	2	-18*	0	17	7	13	-5	12*	0	14	11	13	4	-24*	0	15
2	13	3	-20*	0	16	7	13	-4	20*	0	16	12	13	-4	24*	0	10
2	13	4	20*	0	11	7	13	-3	-41*	0	15	12	13	-3	-31*	0	13
2	13	5	-32*	0	12	7	13	-2	-22*	0	10	12	13	-2	20*	0	18
3	13	-5	25*	0	9	7	13	-1	21*	0	17	12	13	-1	18*	0	11
3	13	-4	-42*	0	11	7	13	0	29*	0	8	12	13	0	-39*	0	11
3	13	-3	19*	0	11	7	13	1	23*	0	9	12	13	1	-26*	0	14
3	13	-2	-14*	0	18	7	13	2	-9*	0	14	12	13	2	-19*	0	15
3	13	-1	-24*	0	13	7	13	3	20*	0	17	12	13	3	-42*	0	10
3	13	0	-8*	0	14	7	13	4	-21*	0	10	13	13	-3	-16*	0	18
3	13	1	-23*	0	16	8	13	-5	-31*	0	13	13	13	-2	-8*	0	15
3	13	2	19*	0	11	8	13	-4	-30*	0	13	13	13	-1	-16*	0	11
3	13	3	-38*	0	21	8	13	-3	31*	0	8	13	13	0	-39*	0	10
3	13	4	12*	0	21	8	13	-2	25*	0	8	13	13	2	9*	0	14
3	13	5	-21*	0	15	8	13	-1	-34*	0	13	13	13	3	-25*	0	9
4	13	-5	24*	0	9	8	13	0	-10*	0	20	14	13	-3	24*	0	17
4	13	-4	18*	0	13	8	13	1	26*	0	8	14	13	-2	21*	0	12
4	13	-3	-11*	0	11	8	13	2	-6*	0	16	14	13	-1	-32*	0	10
4	13	-2	-17*	0	19	8	13	3	-37*	0	7	14	13	0	20*	0	13
4	13	-1	-12*	0	14	8	13	4	-30*	0	13	14	13	1	-25*	0	10
4	13	0	-8*	0	14	8	13	5	-34*	0	12	14	13	2	12*	0	17
4	13	1	42	45	6	9	13	-4	-7*	0	23	15	13	-2	-31*	0	12
4	13	2	21*	0	16	9	13	-3	-22*	0	15	15	13	-1	0*	0	21
4	13	3	-23*	0	12	9	13	-2	-33*	0	12	15	13	0	-17*	0	11
4	13	4	-14*	0	14	9	13	-1	-30*	0	12	15	13	1	-41*	0	12
4	13	5	-25*	0	14	9	13	0	12*	0	13	15	13	2	0*	0	31
5	13	-5	-32*	0	13	9	13	1	-18*	0	15	16	13	-1	-17*	0	11
5	13	-4	-19*	0	17	9	13	2	-15*	0	18	16	13	0	-41*	0	12
5	13	-3	22*	0	10	9	13	3	14*	0	21	16	13	1	-8*	0	23
5	13	-2	24*	0	8	9	13	4	-31*	0	12	0	14	0	-13*	0	19
5	13	-1	-14*	0	7	10	13	-4	-25*	0	15	0	14	1	-10*	0	17
5	13	0	31*	0	19	10	13	-3	-26*	0	10	0	14	2	26*	0	9
5	13	1	11*	0	21	10	13	-2	-23*	0	14	0	14	3	19*	0	17
5	13	2	-21*	0	9	10	13	-1	23*	0	10	0	14	4	19*	0	11
5	13	3	-7*	0	24	10	13	0	23*	0	17	0	14	5	-30*	0	13
5	13	4	-20*	0	16	10	13	1	18*	0	8	0	14	6	-28*	0	8
5	13	5	24*	0	9	10	13	2	27*	0	13	0	14	7	-21*	0	10
6	13	-5	19*	0	18	10	13	3	-26*	0	13	1	14	8	-26*	0	14

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H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
6	14	1	-21*	0	10	1	15	2	19*	0	19	1	15	2	19*	0	19
6	14	2	-28*	0	13	2	15	-2	-39*	0	11	2	15	-2	-39*	0	11
6	14	3	20*	0	10	2	15	-1	-24*	0	16	2	15	-1	-24*	0	16
7	14	-4	23*	0	10	2	15	0	-23*	0	20	2	15	0	-23*	0	20
7	14	-3	-16*	0	19	2	15	1	-16*	0	6	2	15	1	-16*	0	6
7	14	-2	20*	0	17	2	15	2	40*	0	9	2	15	2	40*	0	9
7	14	-1	0*	0	31	3	15	-2	27*	0	6	3	15	-2	27*	0	6
7	14	0	-35*	0	11	3	15	-1	45*	30	6	3	15	-1	45*	30	6
7	14	1	19*	0	18	3	15	0	24*	0	10	3	15	0	24*	0	10
7	14	2	-30*	0	14	3	15	1	-19*	0	19	3	15	1	-19*	0	19
7	14	3	-18*	0	17	3	15	2	-20*	0	18	3	15	2	-20*	0	18
8	14	-3	-42*	0	12	4	15	-2	-42*	0	11	4	15	-2	-42*	0	11
8	14	-2	8*	0	23	4	15	-1	33*	0	8	4	15	-1	33*	0	8
8	14	-1	17*	0	11	4	15	0	23*	0	11	4	15	0	23*	0	11
8	14	0	28*	0	9	4	15	1	26*	0	10	4	15	1	26*	0	10
8	14	1	19*	0	15	4	15	2	20*	0	12	4	15	2	20*	0	12
8	14	2	8*	0	24	5	15	-2	-11*	0	24	5	15	-2	-11*	0	24
8	14	3	-20*	0	9	5	15	-1	19*	0	19	5	15	-1	19*	0	19
9	14	-3	-18*	0	16	5	15	0	-20*	0	11	5	15	0	-20*	0	11
9	14	-2	-16*	0	19	5	15	1	5*	0	20	5	15	1	5*	0	20
9	14	-1	-13*	0	19	5	15	2	38*	0	7	5	15	2	38*	0	7
9	14	0	-11*	0	21	6	15	-2	-16*	0	21	6	15	-2	-16*	0	21
9	14	1	-25*	0	9	6	15	-1	-14*	0	13	6	15	-1	-14*	0	13
9	14	2	-28*	0	14	6	15	0	34*	0	8	6	15	0	34*	0	8
9	14	3	-34*	0	13	6	15	1	5*	0	20	6	15	1	5*	0	20
10	14	-2	-11*	0	13	7	15	-1	32*	0	8	7	15	-1	32*	0	8
10	14	-1	-36*	0	22	7	15	0	41*	23	6	7	15	0	41*	23	6
10	14	0	-38*	0	12	7	15	1	-14*	0	19	7	15	1	-14*	0	19
10	14	1	-19*	0	10	8	15	0	-22*	0	15	8	15	0	-22*	0	15
10	14	2	-32*	0	17	8	15	1				8	15	1			
11	14	-2	-24*	0	16												
11	14	-1	-8*	0	13												
11	14	0	-28*	0	15												
11	14	1	-33*	0	8												
12	14	-2	-41*	0	12												
12	14	-1	15*	0	11												
12	14	0	-44*	0	13												
12	14	1	15*	0	10												
13	14	-1	-18*	0	19												
13	14	0	-11*	0	17												
0	15	1	35*	0	21												
0	15	2	34*	0	8												
1	15	-2	37*	0	10												
1	15	-1	29*	0	7												
1	15	0	24*	0	8												
1	15	1	41*	0	10												
1	15	1		0	7												

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